

## Supporting Information

### **Influence of Molecular Geometry, Exchange-Correlation Functional, and Solvent Effects in the Modeling of Vertical Excitation Energies in Phthalocyanines Using TDDFT and PCM-TDDFT Methods: Can Modern Computational Chemistry Methods Explain Experimental Controversies?**

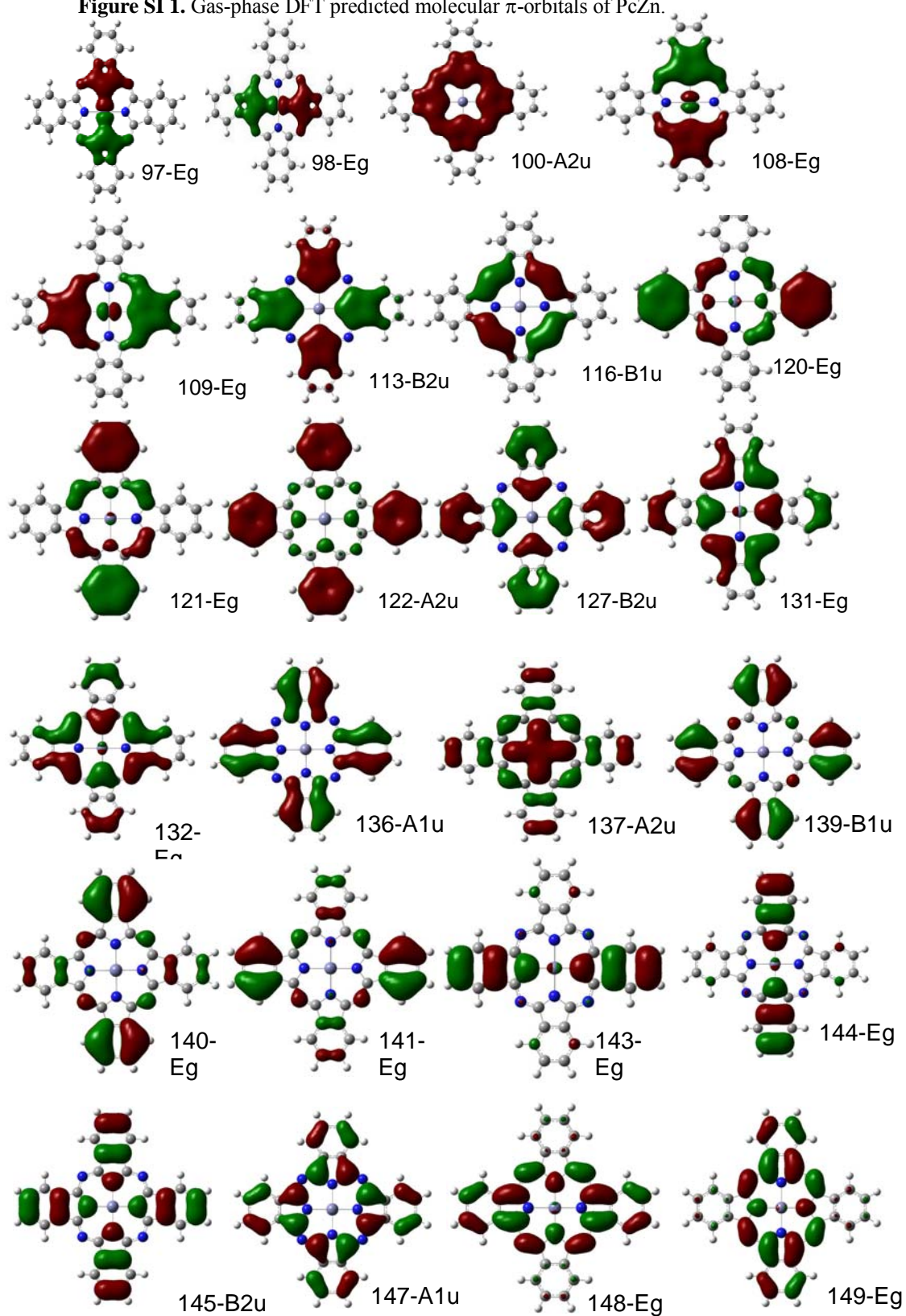
Victor N. Nemykin,<sup>†\*</sup> Ryan G. Hadt,<sup>†</sup> Rodion V. Belosludov,<sup>‡\*</sup> Hiroshi Mizuseki,<sup>‡</sup> and Yoshiyuki Kawazoe<sup>‡</sup>

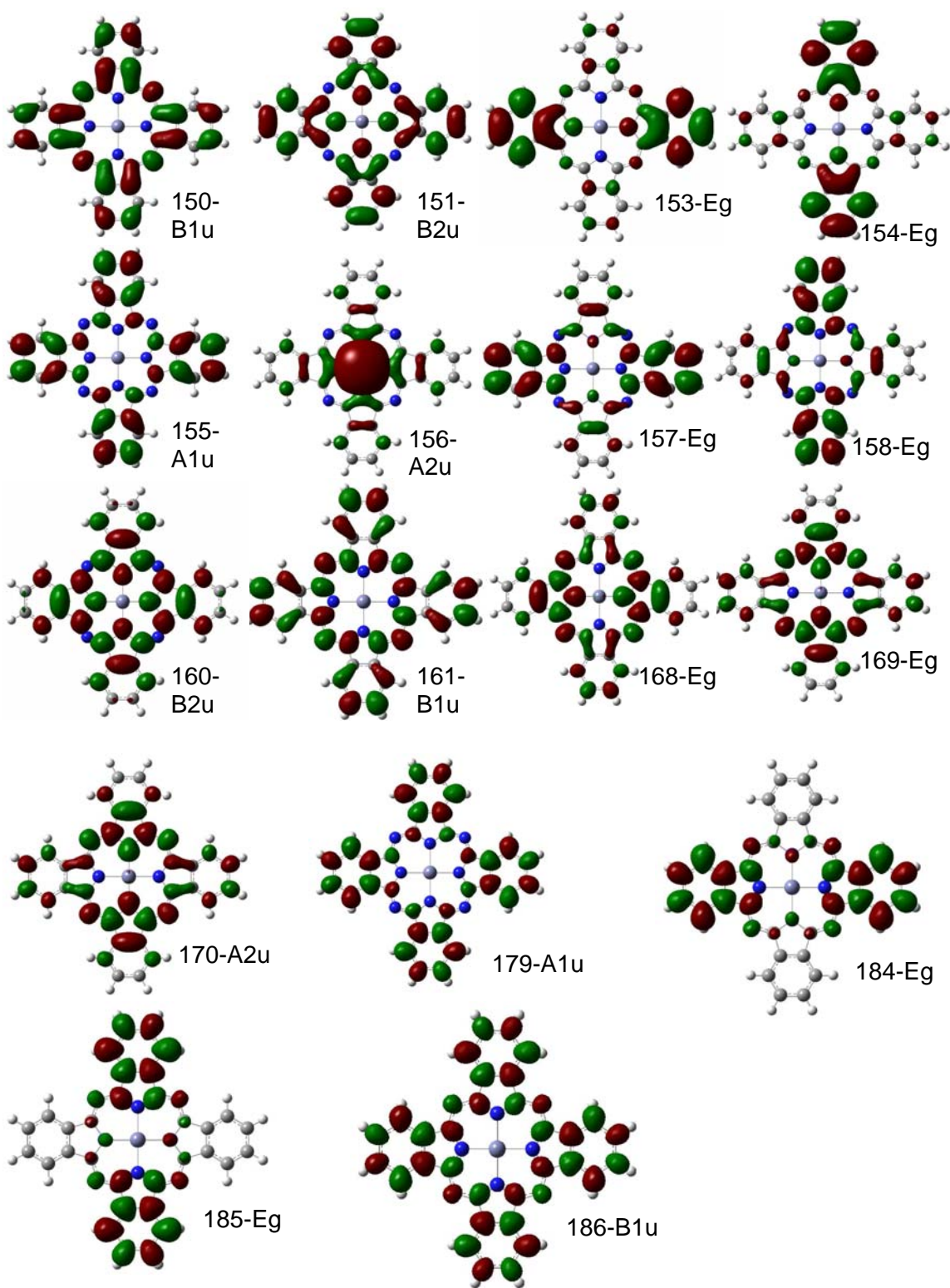
<sup>†</sup>*Department of Chemistry & Biochemistry, University of Minnesota Duluth, Duluth, MN 55812, USA and* <sup>‡</sup>*Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan*

---

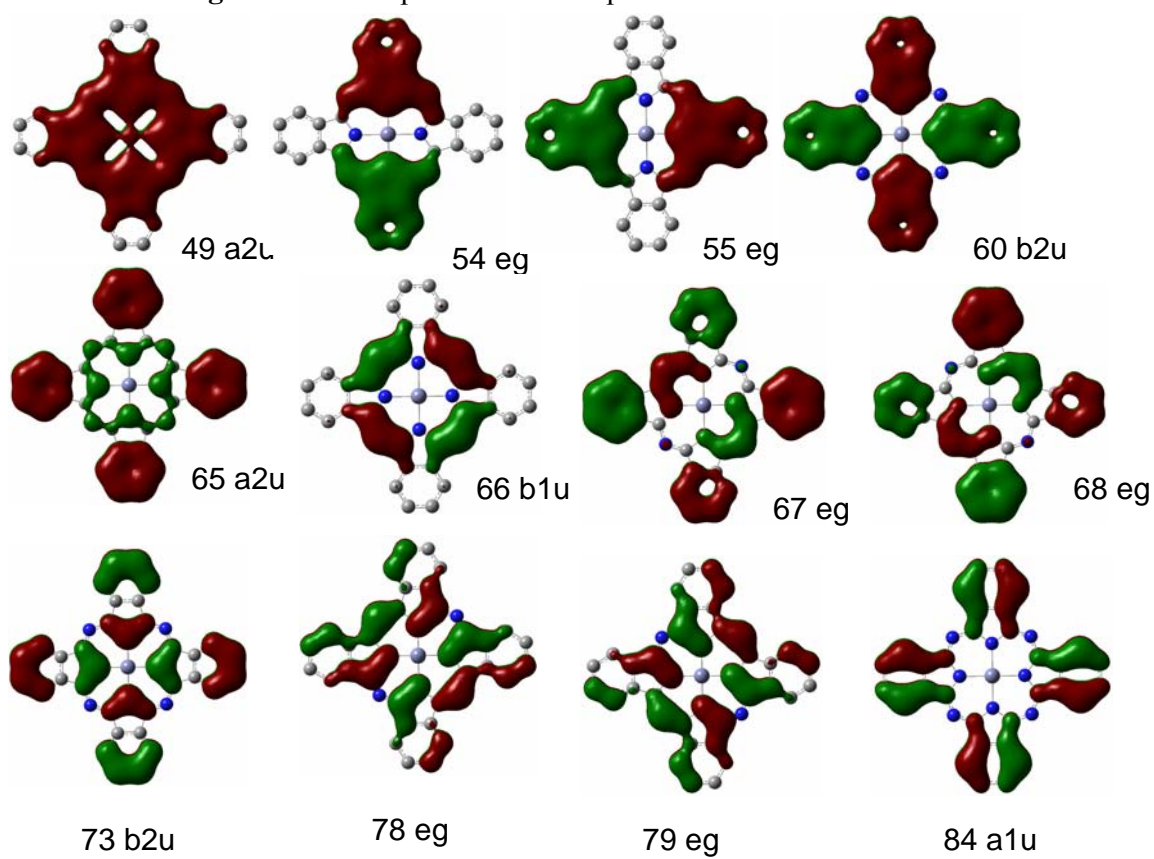
\* author to whom correspondence should be addressed: [vnemykin@d.umn.edu](mailto:vnemykin@d.umn.edu) (VNN), [rodion@imr.edu](mailto:rodion@imr.edu) (RVB)

**Figure SI 1.** Gas-phase DFT predicted molecular  $\pi$ -orbitals of PcZn.

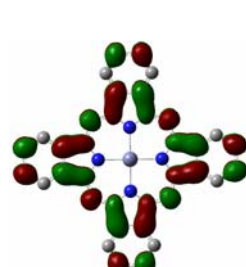
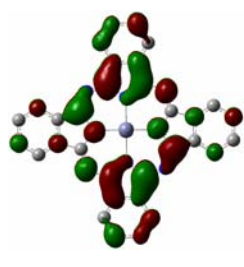
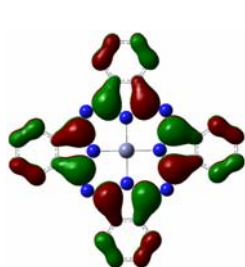
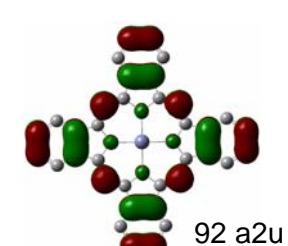
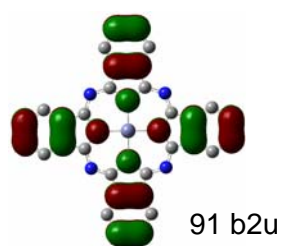
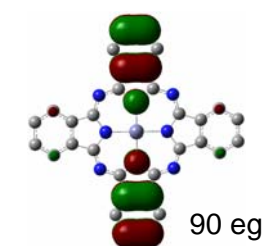
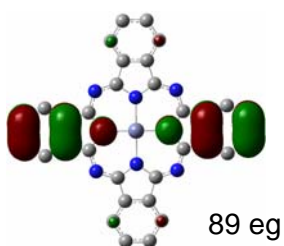
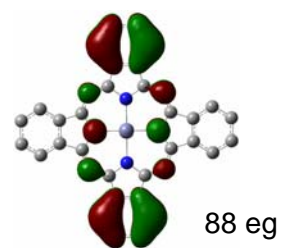
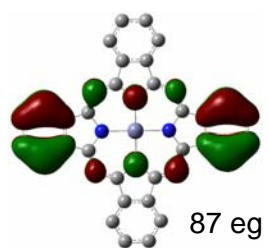
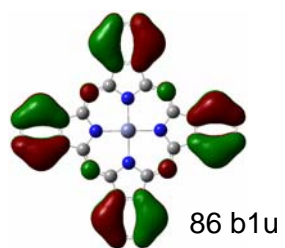
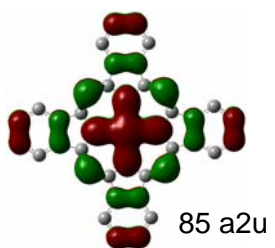


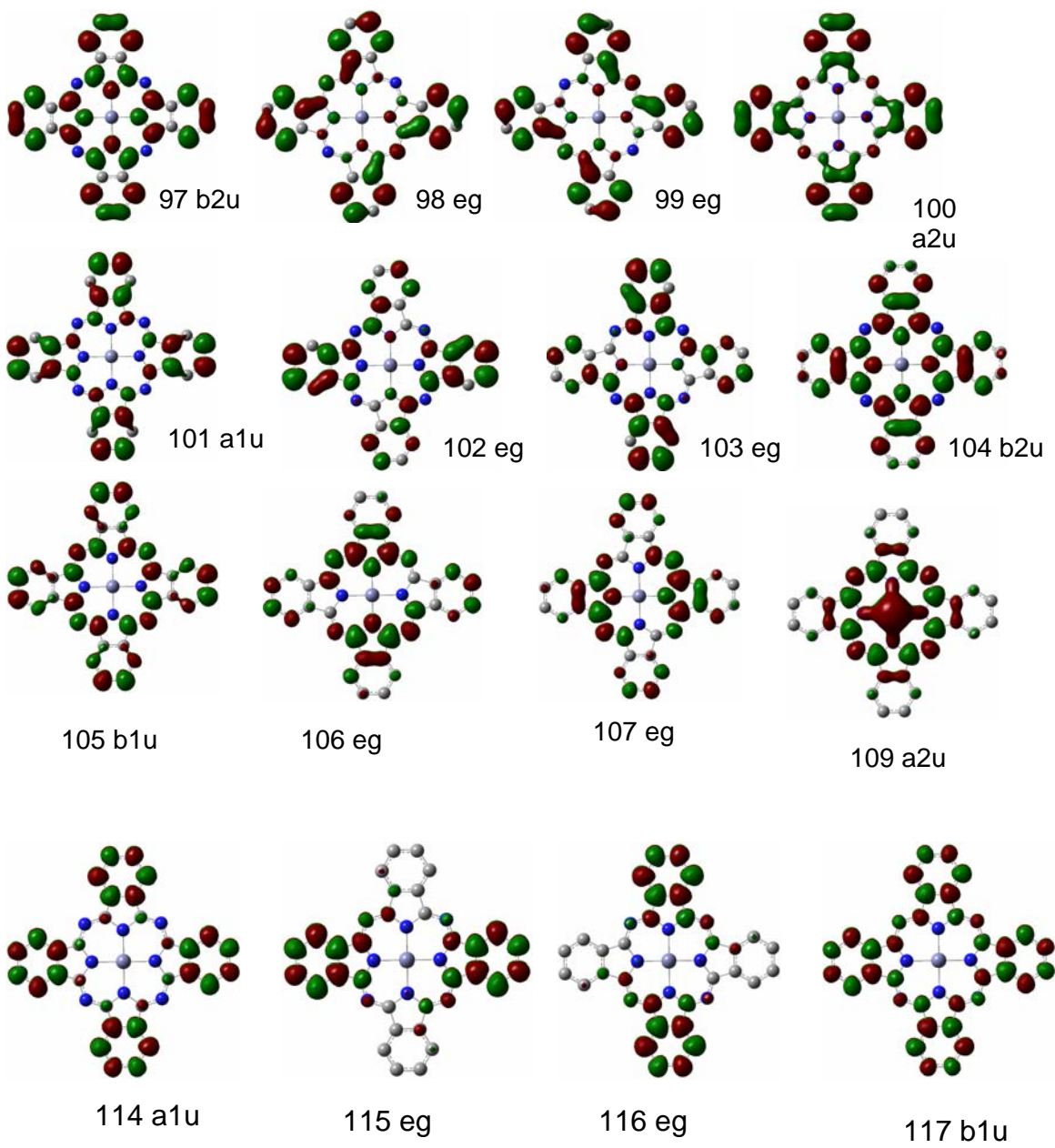


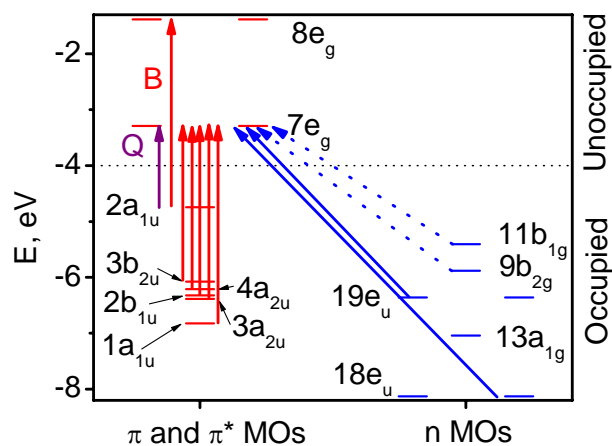
**Figure SI 2.** Gas-phase ZINDO/S predicted molecular  $\pi$ -orbitals of PcZn.



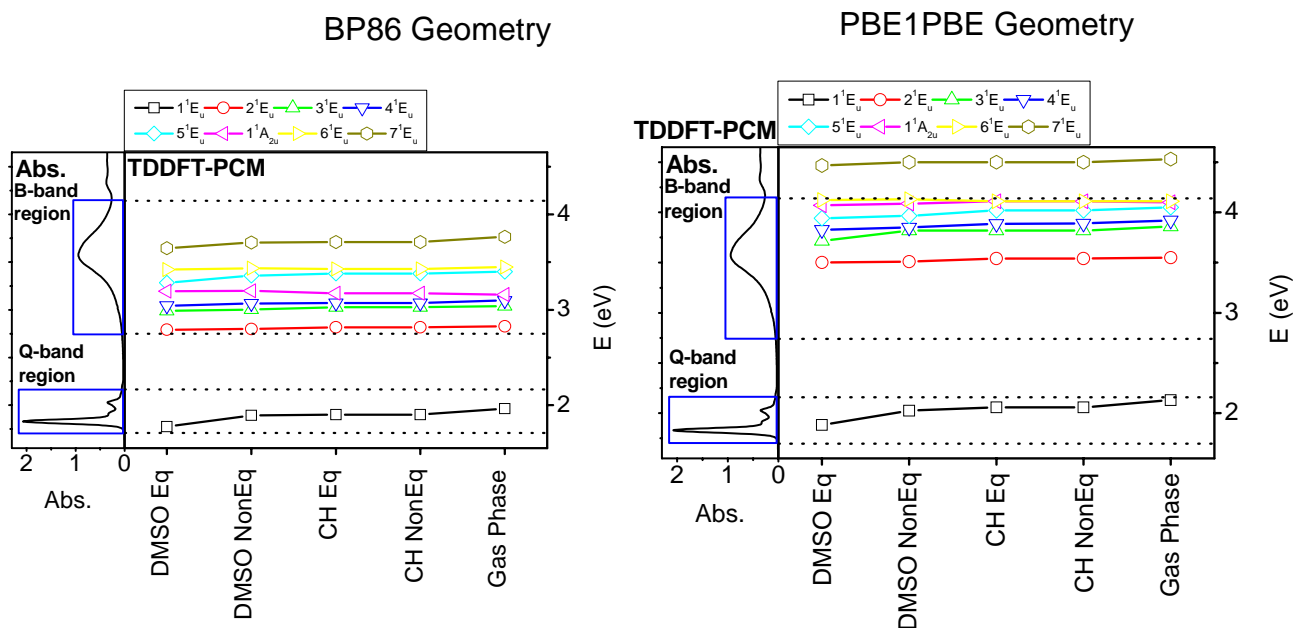








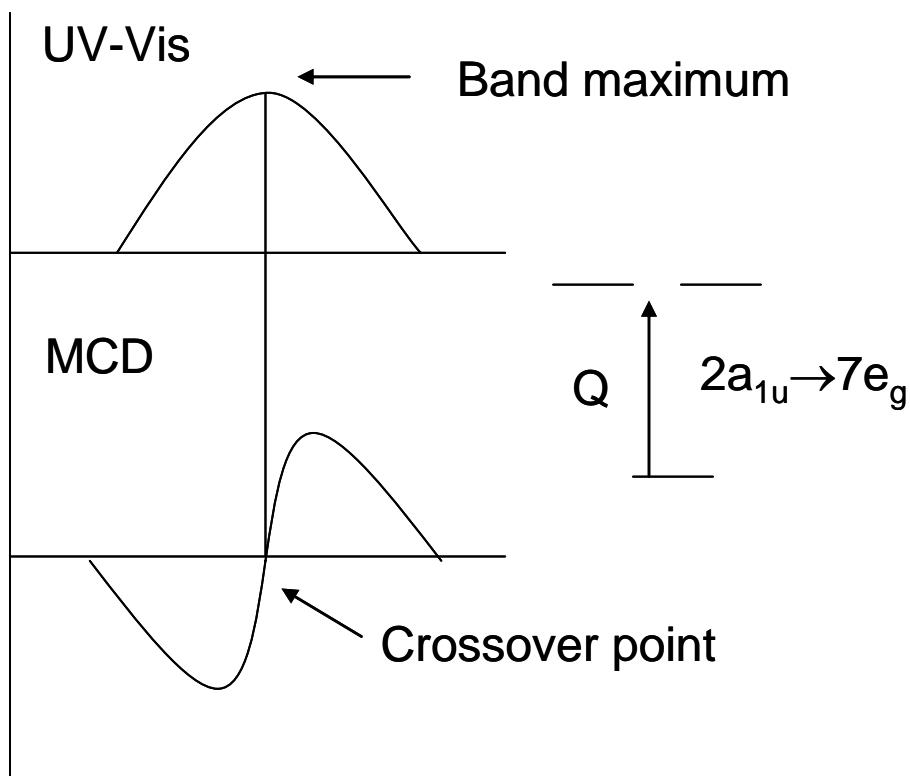
**Figure SI 3.** Simplified overview on the single-electron transitions observed in Q- and B- band spectral envelopes. Symmetry-forbidden  $n \rightarrow \pi^*$  transitions are indicated by dotted lines.



**Figure SI 4.** Gas-phase and PCM-TDDFT predicted vertical excitation energies of PcZn calculated for two different molecular geometries.

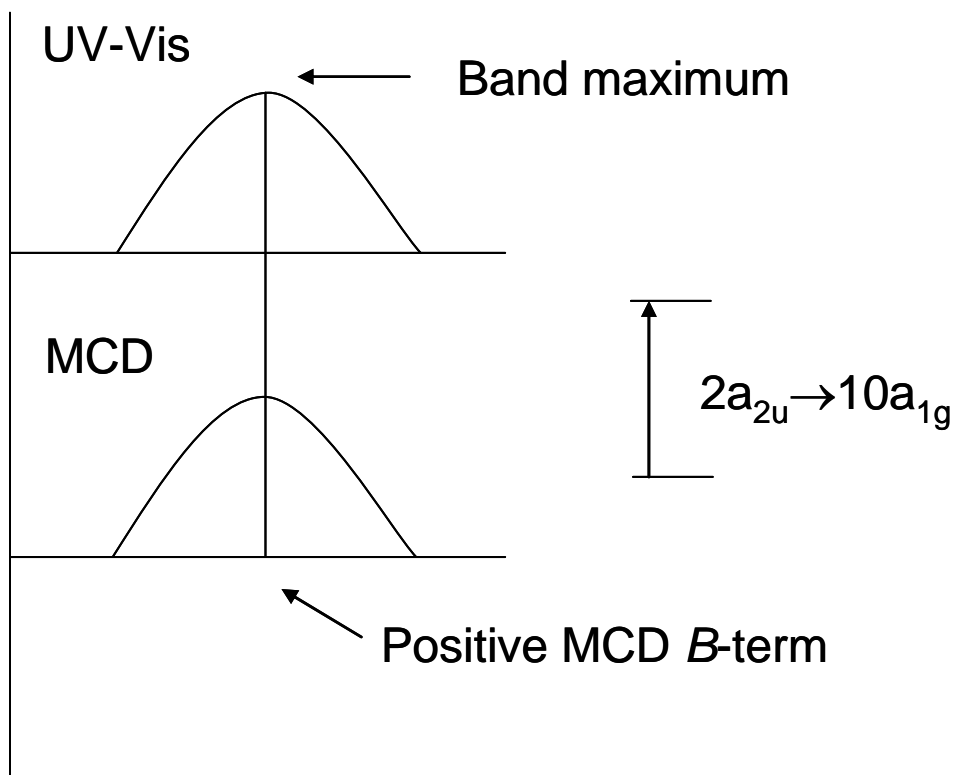
## Faraday A and B terms in MCD spectroscopy in application to PcZn ( $D_{4h}$ symmetry)

In the case of diamagnetic PcZn complex with effective  $D_{4h}$  symmetry, the only Faraday A and B terms are expected in MCD spectra. The Faraday A term appears if the excited states are degenerate (*i.e.*  $^1E_u$  states in the case of PcZn). The crossover point of MCD Faraday A term corresponds to the band maximum in UV-Vis spectrum. For instance, Q band in the UV-Vis spectrum of PcZn predominantly originates from  $2a_{1u} \rightarrow 7e_g$  symmetry allowed transition and results in MCD Faraday A term:





Mixing of an excited state with the nearby transitions by the magnetic field results in MCD Faraday  $B$  terms, which observed as negative or positive amplitude Gaussian-shaped bands. The maximum (positive or negative) amplitude in MCD Faraday  $B$  term corresponds to the maximum amplitude in respective UV-Vis band. In the case of PcZn (if selected rules allowed), all excitations from non-degenerate to non-degenerate MOs will result in MCD Faraday  $B$  terms:



**Supporting Information Table 1.** Comparison between X-ray crystallographically determined and solution optimized bond distances and angles in PcZn.

from a	Data							
	Method/media	Zn-N	N-C <sub>α</sub>	C <sub>α</sub> -N <sub>meso</sub>	C <sub>α</sub> -C <sub>β</sub>	C <sub>β</sub> -C <sub>β</sub>	C <sub>α</sub> -N <sub>Zn</sub> -C <sub>α</sub>	C <sub>α</sub> -N <sub>meso</sub> -C <sub>α</sub>
	BP86/cyclohexane	1.993	1.384	1.339	1.466	1.420	109.0	123.8
	BP86/DMSO	1.998	1.382	1.341	1.468	1.421	109.1	123.9
	B3LYP/cyclohexane	1.996	1.373	1.331	1.461	1.411	109.6	124.5
	B3LYP/benzene	1.994	1.372	1.331	1.461	1.411	109.5	124.4
	B3LYP/dichloromethane	1.997	1.372	1.332	1.463	1.412	109.6	124.6
	B3LYP/DMSO	1.991	1.373	1.330	1.461	1.410	109.4	124.3
	PBE1PBE/cyclohexane	1.982	1.366	1.326	1.457	1.405	109.4	124.1
	PBE1PBE/DMSO	2.012	1.364	1.327	1.458	1.406	109.2	124.0
	Exp <sup>a</sup>	1.980(2)	1.369(2)	1.331(2)	1.455(2)	1.400(3)	109.1(2)	123.5(2)

reference 52. The numbers in parentheses are estimated standard deviations.

**Supporting Information Table 2.** Calculated molecular orbital energies and compositions of PcZn using 14 exchange-correlation functionals and gas-phase molecular geometry calculated using B3LYP exchange-correlation functional.

**X $\alpha$  Exchange Correlation Functional**

Orbital	Index	E, eV	Zn	N <sub>pyrr</sub>	N <sub>meso</sub>	Pc	Total
	1 A1G)--O	-9398.42	100	0	0	0	100
	2 (A1G)--O	-1133.21	100	0	0	0	100
	3 (A2U)--O	-1001.02	100	0	0	0	100
	4 (EU)--O	-1000.84	100	0	0	0	100
	5 (EU)--O	-1000.84	100	0	0	0	100
	6 (EU)--O	-378.396	0	99.8	0	0.1	100
	7 (EU)--O	-378.396	0	99.8	0	0.1	100
	8 (B1G)--O	-378.396	0	99.8	0	0.2	100
	9 (A1G)--O	-378.396	0	99.9	0	0.1	100
	10 (EU)--O	-378.055	0	0	99.7	0.2	100
	11 (EU)--O	-378.055	0	0	99.7	0.2	100
	12 (B2G)--O	-378.055	0	0	99.7	0.3	100
	13 (A1G)--O	-378.054	0	0	99.8	0.2	100
	14 (EU)--O	-268.408	0	0	0.1	99.9	100
	15 (EU)--O	-268.408	0	0	0.1	99.9	100
	16 B2G)--O	-268.408	0	0	0.2	99.8	100
	17 (A1G)--O	-268.408	0	0.1	0	99.9	100
	18 (A2G)--O	-268.407	0	0	0	100	100
	19 (EU)--O	-268.407	0	0	0	99.9	100
	20 (EU)--O	-268.407	0	0	0	99.9	100
	21 B1G)--O	-268.406	0	0	0	100	100
	22 (EU)--O	-266.653	0	0	0	100	100
	23 (EU)--O	-266.653	0	0	0	100	100
	24 (A1G)--O	-266.653	0	0	0	100	100
	25 (B1G)--O	-266.653	0	0	0	100	100
	26 A2G)--O	-266.649	0	0	0	100	100
	27 (EU)--O	-266.649	0	0	0	100	100
	28 (EU)--O	-266.649	0	0	0	100	100
	29 (B2G)--O	-266.649	0	0	0	100	100
	30 (A2G)--O	-266.605	0	0	0	100	100
	31 (EU)--O	-266.605	0	0	0	100	100
	32 (EU)--O	-266.605	0	0	0	100	100
	33 (B2G)--O	-266.605	0	0	0	100	100
	34 (B1G)--O	-266.605	0	0	0	100	100
	35 (EU)--O	-266.605	0	0	0	100	100
	36 (EU)--O	-266.605	0	0	0	100	100
	37 (A1G)--O	-266.605	0	0	0	100	100
	38 (B1G)--O	-266.591	0	0	0	100	100
	39 (EU)--O	-266.591	0	0	0	100	100

40 (EU)--O	-266.591	0	0	0	100	100
41 A1G)--O	-266.591	0	0	0	100	100
42 (A2G)--O	-266.587	0	0	0	100	100
43 (EU)--O	-266.587	0	0	0	100	100
44 (EU)--O	-266.587	0	0	0	100	100
45 (B2G)--O	-266.587	0	0	0	100	100
46 A1G)--O	-123.673	100	0	0	0	100
47 (A2U)--O	-81.64	100	0	0	0	100
48 (EU)--O	-81.331	100	0	0	0	100
49 (EU)--O	-81.331	100	0	0	0	100
50 (A1G)--O	-24.182	0.5	39.9	24.4	35.2	100
51 (EU)--O	-23.814	0.2	39.2	23.7	37	100
52 (EU)--O	-23.814	0.2	39.2	23.7	37	100
53 (B1G)--O	-23.113	0.1	58.4	0.8	40.7	100
54 (B2G)--O	-22.513	0	1.9	68.5	29.5	100
55 (EU)--O	-21.482	0	17.3	49.6	33.1	100
56 (EU)--O	-21.482	0	17.3	49.6	33.1	100
57 (A1G)--O	-20.683	0.1	16.8	49.9	33.1	100
58 (A1G)--O	-20.199	0.4	20	6.6	73	100
59 (EU)--O	-20.175	0.1	13.9	1.1	84.9	100
60 (EU)--O	-20.175	0.1	13.9	1.1	84.9	100
61 B1G)--O	-20.159	0.1	12.6	0	87.3	100
62 (A2G)--O	-18.14	0	3.3	7.5	89.2	100
63 (A1G)--O	-17.816	0.8	12.7	0.3	86.2	100
64 (EU)--O	-17.775	0.1	14.3	4.4	81.2	100
65 (EU)--O	-17.775	0.1	14.3	4.4	81.2	100
66 (EU)--O	-17.654	0	3.8	1.5	94.7	100
67 (EU)--O	-17.654	0	3.8	1.5	94.7	100
68 (B1G)--O	-17.647	0.4	19	0.7	79.8	100
69 (B2G)--O	-17.561	0	0	1.7	98.2	100
70 (A2G)--O	-16.791	0	5.6	8.3	86.1	100
71 (EU)--O	-16.182	0	6.8	18.2	75	100
72 (EU)--O	-16.182	0	6.8	18.2	75	100
73 (B1G)--O	-14.87	0.5	8.1	23.7	67.7	100
74 (A1G)--O	-14.715	2.5	11.9	0.7	84.8	100
75 (EU)--O	-14.534	0.3	11.4	0.6	87.7	100
76 (EU)--O	-14.534	0.3	11.4	0.6	87.7	100
77 (B2G)--O	-14.358	0.1	3.5	14.5	82	100
78 (B1G)--O	-14.334	1	9.2	6.7	83.2	100
79 (B2G)--O	-13.719	1.6	30	22.4	46	100
80 (EU)--O	-13.684	0.1	7.4	3	89.5	100
81 (EU)--O	-13.684	0.1	7.4	3	89.5	100
82 (A2G)--O	-13.424	0	6.7	1.4	91.9	100
83 (A1G)--O	-12.743	3.3	7.8	1.4	87.6	100
84 (EU)--O	-12.613	0	19.7	17	63.2	100
85 (EU)--O	-12.613	0	19.7	17	63.2	100
86 (EU)--O	-12.244	0.4	10.1	15.2	74.3	100
87 (EU)--O	-12.244	0.4	10.1	15.2	74.3	100
88 (B1G)--O	-12.175	6.1	12.9	5.1	76	100
89 (A2G)--O	-11.491	0	20.7	13.8	65.5	100
90 (B2G)--O	-11.249	0.9	1.6	1.5	96.1	100

91 A1G)--O	-11.011	22.3	20.6	2.2	55	100
92 (B1G)--O	-10.797	35.7	18.4	0.3	45.6	100
93 (EU)--O	-10.77	0	3	3.9	93.1	100
94 (EU)--O	-10.77	0	3	3.9	93.1	100
95 (A2U)--O	-10.598	0.6	25.1	17.7	56.6	100
96 (EU)--O	-10.425	0.7	13.1	1.8	84.3	100
97 (EU)--O	-10.425	0.7	13.1	1.8	84.3	100
98 (EG)--O	-10.307	19.3	24.5	11.9	44.2	100
99 (EG)--O	-10.307	19.3	24.5	11.9	44.2	100
100 (A2G)--O	-10.235	0	1	6.7	92.3	100
101 A1G)--O	-9.964	10.2	9.8	6.3	73.6	100
102 (B1G)--O	-9.924	20.7	10.8	1.9	66.7	100
103 (EU)--O	-9.715	0.1	1.6	1.5	96.9	100
104 (EU)--O	-9.715	0.1	1.6	1.5	96.9	100
105 (B2G)--O	-9.697	0.3	0.1	0.6	99	100
106 A1G)--O	-9.591	41.2	3.5	2.2	53.1	100
107 (B2U)--O	-9.468	0	26.4	0	73.5	100
108 (A2G)--O	-9.467	0	0.6	3.2	96.1	100
109 (EU)--O	-9.402	0.4	5.5	4.1	90	100
110 (EU)--O	-9.402	0.4	5.5	4.1	90	100
111 (EG)--O	-9.266	88.1	1.1	2	8.8	100
112 (EG)--O	-9.266	88.1	1.1	2	8.8	100
113 (B2G)--O	-9.207	49.8	6.6	0.9	42.7	100
114 (B1G)--O	-9.023	14.8	0.9	3.2	81.1	100
115 (A1G)--O	-8.612	60.8	11.6	2.7	24.9	100
116 B1U)--O	-8.609	0	0	50.3	49.7	100
117 (EG)--O	-8.069	2.1	1.8	15.2	80.9	100
118 (EG)--O	-8.069	2.1	1.8	15.2	80.9	100
119 (A2U)--O	-8.045	0.4	7	3.9	88.7	100
120 (B2G)--O	-7.94	0.8	0.1	1.4	97.7	100
121 (EU)--O	-7.873	0.1	1.7	1.8	96.5	100
122 (EU)--O	-7.873	0.1	1.7	1.8	96.5	100
123 (A2G)--O	-7.698	0	1.7	0.9	97.4	100
124 (B2U)--O	-7.66	0	25.3	0	74.7	100
125 (EU)--O	-7.596	6.2	37.4	2.8	53.6	100
126 (EU)--O	-7.596	6.2	37.4	2.8	53.6	100
127 (A1G)--O	-7.513	0	2.1	3	94.9	100
128 (EU)--O	-7.215	1.9	10.5	5.7	82	100
129 (EU)--O	-7.215	1.9	10.5	5.7	82	100
130 (B1G)--O	-7.178	1.4	0.6	2.7	95.3	100
131 (EG)--O	-7.006	3.2	19.5	20	57.3	100
132 (EG)--O	-7.006	3.2	19.5	20	57.3	100
133 (A1G)--O	-6.112	0.1	20.2	50.7	29	100
134 (A1U)--O	-6	0	0	0	99.9	100
135 (A2U)--O	-5.582	3.5	48.1	27.2	21.2	100
136 B1U)--O	-5.495	0	0	5.3	94.7	100
137 (EG)--O	-5.476	0	0.4	10	89.6	100
138 (EG)--O	-5.476	0	0.4	10	89.6	100
139 (EU)--O	-5.459	0.2	18	47.4	34.4	100
140 (EU)--O	-5.459	0.2	18	47.4	34.4	100
141 A2U)--O	-5.391	0	2.6	33.9	63.5	100



142 (EG)--O	-5.265	2	28.6	1.6	67.8	100
143 (EG)--O	-5.265	2	28.6	1.6	67.8	100
144 (B2U)--O	-5.25	0	26	0	74	100
145 (B2G)--O	-4.994	0.6	11.5	58.3	29.6	100
146 B1G)--O	-4.549	23.6	48.5	0.8	27.1	100
147 (A1U)--O	-3.944	0	0.1	0.1	99.8	100
148 (EG)--V	-2.489	0.4	13.3	19.9	66.3	100
149 (EG)--V	-2.489	0.4	13.3	19.9	66.3	100
150 (B1U)--V	-1.063	0	0	25.4	74.6	100
151 B2U)--V	-0.846	0	19.7	0	80.3	100
152 (A2U)--V	-0.751	8.3	0.7	5.8	85.1	100
153 (EG)--V	-0.579	0.1	5.6	3.7	90.6	100
154 (EG)--V	-0.579	0.1	5.6	3.7	90.6	100
155 (A1U)--V	0.597	0	0	0	100	100
156 (EG)--V	0.653	0	1.7	0.9	97.3	100
157 (EG)--V	0.653	0	1.7	0.9	97.3	100
158 (A2U)--V	0.694	60.9	8.9	1.7	28.5	100
159 (A1G)--V	0.933	72.7	16.5	0.3	10.5	100
160 (B2U)--V	1.203	0	19.4	0.1	80.5	100
161 B1U)--V	1.395	0	0.1	18.5	81.5	100
162 (EU)--V	2.576	47.8	6.1	2.5	43.5	100
163 (EU)--V	2.576	47.8	6.1	2.5	43.5	100
164 (A1G)--V	2.619	0.2	0.1	1.9	97.9	100
165 (EG)--V	2.678	0.1	14.5	16	69.4	100
166 (EG)--V	2.678	0.1	14.5	16	69.4	100
167 (EU)--V	2.796	24	2.6	0.4	72.9	100
168 (EU)--V	2.796	24	2.6	0.4	72.9	100
169 (B1G)--V	2.81	0	0	0.1	99.9	100
170 (A2U)--V	3.27	30.8	15.5	16	37.6	100
171 B2G)--V	3.597	0	1	0.1	98.9	100
172 (EU)--V	3.802	0	1.1	0.2	98.6	100
173 (EU)--V	3.802	0	1.1	0.2	98.6	100
174 (A1G)--V	3.802	37.3	0.6	11.4	50.7	100
175 (A2G)--V	4.058	0	0.7	0.1	99.3	100
176 A1U)--V	4.32	0	0	0	100	100
177 (EU)--V	4.487	1.1	0.1	3.7	95.1	100
178 (EU)--V	4.487	1.1	0.1	3.7	95.1	100
179 (EG)--V	4.49	0	0.9	4	95.1	100
180 (EG)--V	4.49	0	0.9	4	95.1	100
181 B1U)--V	4.508	0	0	4.6	95.4	100
182 (B2G)--V	4.515	0	0.1	6	93.9	100
183 (A1G)--V	4.696	27.8	0.9	0.1	71.2	100
184 (B1G)--V	4.859	0	5.7	0.3	94	100
185 (EU)--V	4.875	1.2	2.5	0.3	96	100
186 (EU)--V	4.875	1.2	2.5	0.3	96	100
187 (A2G)--V	5.087	0	0.1	0.1	99.8	100
188 (B2G)--V	5.549	0.1	3	11.7	85.2	100
189 (EU)--V	5.557	5	8.8	3.9	82.2	100
190 (EU)--V	5.557	5	8.8	3.9	82.2	100
191 A1G)--V	5.806	0.1	0.8	1.5	97.6	100
192 (B1G)--V	5.807	0	27.7	3.4	68.9	100

193 (A2U)--V	6.107	87.2	3.3	1.2	8.2	100
194 (EU)--V	6.352	0.1	0.7	1.4	97.8	100
195 (EU)--V	6.352	0.1	0.7	1.4	97.8	100
196 A2G)--V	6.411	0	6.1	0.6	93.3	100
197 (EU)--V	6.695	1.1	0.3	6.5	92.2	100
198 (EU)--V	6.695	1.1	0.3	6.5	92.2	100
199 (B2G)--V	6.757	0	0.4	11.4	88.2	100
200 (B1G)--V	7.012	0	2.8	0	97.2	100
201 A2G)--V	7.022	0	0.2	0	99.8	100
202 (A1G)--V	7.29	8.7	10	21.2	60.2	100
203 (EU)--V	7.335	1.6	5.9	2.3	90.2	100
204 (EU)--V	7.335	1.6	5.9	2.3	90.2	100
205 (EU)--V	7.675	0.9	6.6	2.8	89.7	100
206 (EU)--V	7.675	0.9	6.6	2.8	89.7	100
207 (A1G)--V	7.8	4.8	0.6	2.8	91.9	100
208 (B2G)--V	8.418	0	0.7	3.9	95.4	100
209 (B1G)--V	8.421	0	0.4	0.1	99.5	100
210 (EU)--V	8.71	0.3	2.9	14.2	82.5	100
211 (EU)--V	8.71	0.3	2.9	14.2	82.5	100
212 (EU)--V	8.946	2.1	3.8	0.4	93.6	100
213 (EU)--V	8.946	2.1	3.8	0.4	93.6	100
214 (A1G)--V	8.96	0.2	2	2.8	95.1	100
215 (B2G)--V	9.15	0	4.5	24.8	70.7	100
216 B1G)--V	9.499	0	4.3	0.1	95.6	100
217 (B2G)--V	9.705	0	1.1	12.3	86.6	100
218 (A2G)--V	10.045	0	7.1	8.9	84	100
219 (EU)--V	10.077	2.7	3.7	17.4	76.1	100
220 (EU)--V	10.077	2.7	3.7	17.4	76.1	100
221 A1G)--V	10.127	1	16.4	12.8	69.8	100
222 (EU)--V	10.89	2.8	11.5	7	78.7	100
223 (EU)--V	10.89	2.8	11.5	7	78.7	100
224 (A2G)--V	10.99	0	0	0.6	99.4	100
225 (EU)--V	11.104	0.8	1.4	3.8	94	100
226 (EU)--V	11.104	0.8	1.4	3.8	94	100
227 (B1G)--V	11.108	0	19.2	7.8	73	100
228 (EU)--V	12.764	2.4	4.3	4.2	89	100
229 (EU)--V	12.764	2.4	4.3	4.2	89	100
230 (A2G)--V	12.94	0	0.3	7	92.7	100
231 (EG)--V	13.048	0	1.5	1.4	97	100
232 (EG)--V	13.048	0	1.5	1.4	97	100
233 (B2U)--V	13.27	0	0.4	0	99.6	100
234 (B2G)--V	13.286	0	0.4	0.1	99.5	100
235 (A2U)--V	13.382	3.9	0.2	0.7	95.2	100
236 (EG)--V	13.911	0	2.2	1.6	96.2	100
237 (EG)--V	13.911	0	2.2	1.6	96.2	100
238 (EU)--V	13.959	0.1	0.6	3.9	95.4	100
239 (EU)--V	13.959	0.1	0.6	3.9	95.4	100
240 (A1G)--V	14.14	0.7	3.1	0.9	95.3	100
241 B1U)--V	14.201	0	0	4.5	95.5	100
242 (A2G)--V	14.255	0	1.1	3.2	95.6	100
243 (B2G)--V	14.425	0	0.5	2.9	96.6	100

244 (B1G)--V	14.49	0	33.9	5.2	61	100
245 (EU)--V	14.625	0.2	0.3	0.2	99.2	100
246 (EU)--V	14.625	0.2	0.3	0.2	99.2	100
247 (B2U)--V	14.74	0	1.3	0.1	98.6	100
248 (B1G)--V	14.769	0	2.6	2.8	94.6	100
249 (EU)--V	14.827	0	0.4	0.6	99	100
250 (EU)--V	14.827	0	0.4	0.6	99	100
251 A2U)--V	14.849	10.4	1.4	1.4	86.8	100
252 (B2G)--V	14.981	0	0.6	1.5	97.9	100
253 (EG)--V	15.052	0	0.5	1.8	97.7	100
254 (EG)--V	15.052	0	0.5	1.8	97.7	100
255 (A2G)--V	15.133	0	0.2	0.7	99.2	100
256 A1G)--V	15.187	1.8	2.3	17.9	78	100
257 (A1U)--V	15.209	0	0	0	100	100
258 (EU)--V	15.364	0.1	1.3	2.4	96.2	100
259 (EU)--V	15.364	0.1	1.3	2.4	96.2	100
260 (B1G)--V	15.401	0	25	0.9	74.1	100
261 A1G)--V	15.809	1.1	0.2	12.5	86.2	100
262 (EU)--V	15.892	0.3	15.8	16.6	67.3	100
263 (EU)--V	15.892	0.3	15.8	16.6	67.3	100
264 (B1U)--V	16.005	0	0	1	99	100
265 (A2G)--V	16.078	0	0.8	1.9	97.3	100
266 B2G)--V	16.17	0	1	14.2	84.8	100
267 (A1G)--V	16.19	0.8	23.3	9.8	66.1	100
268 (EG)--V	16.203	0	3.9	0.5	95.6	100
269 (EG)--V	16.203	0	3.9	0.5	95.6	100
270 (EU)--V	16.226	0.1	0.4	0.9	98.7	100
271 (EU)--V	16.226	0.1	0.4	0.9	98.7	100
272 (B1G)--V	16.24	0	1.9	0.7	97.4	100
273 (A1G)--V	16.402	0.3	17.1	15.8	66.8	100
274 (EU)--V	16.457	1.6	21.1	9.2	68.2	100
275 (EU)--V	16.457	1.6	21.1	9.2	68.2	100
276 A2G)--V	16.538	0	0.8	2.8	96.4	100
277 (EU)--V	16.805	0.9	3.5	4.1	91.5	100
278 (EU)--V	16.805	0.9	3.5	4.1	91.5	100
279 (EU)--V	16.826	1.8	2.3	9.7	86.3	100
280 (EU)--V	16.826	1.8	2.3	9.7	86.3	100
281 (EG)--V	16.873	0	1.3	3.7	95	100
282 (EG)--V	16.873	0	1.3	3.7	95	100
283 (A2U)--V	16.91	2.9	1.2	1.3	94.6	100
284 (B2G)--V	16.974	0	0.7	13.2	86.1	100
285 (B2U)--V	17.017	0	1.8	0	98.2	100
286 A1U)--V	17.092	0	0	0	100	100
287 (B1G)--V	17.211	0.1	14.5	7.5	78	100
288 (B1U)--V	17.781	0	0	2.3	97.6	100
289 (EG)--V	17.898	0	0.6	0.3	99.1	100
290 (EG)--V	17.898	0	0.6	0.3	99.1	100
291 A2U)--V	18.067	0.7	0.4	4.3	94.7	100
292 (A1G)--V	18.153	5.8	23.8	3.6	66.7	100
293 (B2U)--V	19.357	0	1.1	0	98.9	100
294 (EG)--V	19.401	0	1.7	1.8	96.5	100

295 (EG)--V	19.401	0	1.7	1.8	96.5	100
296 A1U)--V	19.609	0	0	0	100	100
297 (EU)--V	19.716	5.6	15.7	7.1	71.6	100
298 (EU)--V	19.716	5.6	15.7	7.1	71.6	100
299 (B1U)--V	20.163	0	0	3.4	96.6	100
300 (EG)--V	20.555	0.3	36.5	6.8	56.4	100
301 (EG)--V	20.555	0.3	36.5	6.8	56.4	100
302 (B2G)--V	20.855	0	0.1	3	96.9	100
303 (EU)--V	21.07	0.1	1	1.4	97.6	100
304 (EU)--V	21.07	0.1	1	1.4	97.6	100
305 (A1G)--V	21.27	0	0.3	0.8	98.9	100
306 A2U)--V	21.319	1.2	12.4	54.9	31.5	100
307 (B2G)--V	21.487	0	3.3	3.1	93.5	100
308 (EG)--V	21.739	0	1.6	0.4	97.9	100
309 (EG)--V	21.739	0	1.6	0.4	97.9	100
310 (A2G)--V	21.786	0	0.4	0.5	99.1	100
311 (EU)--V	21.92	0.1	0.1	1.2	98.6	100
312 (EU)--V	21.92	0.1	0.1	1.2	98.6	100
313 (A2G)--V	22.298	0	1.5	1.7	96.8	100
314 (EU)--V	22.411	0	0.9	0.5	98.5	100
315 (EU)--V	22.411	0	0.9	0.5	98.5	100
316 B2G)--V	22.435	0	8.1	5.9	85.9	100
317 (B1G)--V	22.466	0	1.2	0.6	98.2	100
318 (B2G)--V	22.921	0	0.7	6.1	93.2	100
319 (A1G)--V	22.966	0.4	8.9	7.2	83.5	100
320 (EU)--V	23.028	0.1	1.9	3.4	94.5	100
321 (EU)--V	23.028	0.1	1.9	3.4	94.5	100
322 (B2U)--V	23.108	0	67.8	0	32.2	100
323 (A2G)--V	23.242	0	0.6	9.5	89.9	100
324 (A1U)--V	23.316	0	0	0	100	100
325 (EU)--V	23.643	0.1	0.8	3.5	95.7	100
326 (EU)--V	23.643	0.1	0.8	3.5	95.7	100
327 (B1G)--V	23.664	0	0.2	0.3	99.5	100
328 (A1G)--V	23.76	2.9	3.3	28.9	64.9	100
329 (EG)--V	23.914	0.1	14.4	41.1	44.5	100
330 (EG)--V	23.914	0.1	14.4	41.1	44.5	100
331 B1U)--V	23.94	0	0	63.5	36.5	100
332 (B1G)--V	24.301	0	20.6	9.9	69.5	100
333 (EU)--V	24.326	0.4	3.7	8.8	87.1	100
334 (EU)--V	24.326	0.4	3.7	8.8	87.1	100
335 (A1G)--V	24.418	0.7	9.2	5.3	84.8	100
336 (EU)--V	24.874	0.3	8.5	4.7	86.4	100
337 (EU)--V	24.874	0.3	8.5	4.7	86.4	100
338 (A2G)--V	25.045	0	0	0	99.9	100
339 (B1G)--V	25.084	0	0.3	0.4	99.3	100
340 (EU)--V	25.496	0.3	0.1	3.3	96.3	100
341 (EU)--V	25.496	0.3	0.1	3.3	96.3	100
342 (B2G)--V	25.955	0	0	0.5	99.5	100
343 (A2G)--V	25.966	0	0	1.8	98.2	100
344 (A2U)--V	26.009	4.6	42.4	16.1	37	100
345 (EU)--V	26.115	0	0.8	2.4	96.8	100

346 (EU)--V	26.115	0	0.8	2.4	96.8	100
347 (B2G)--V	26.602	0	1.4	2.6	96	100
348 (B1G)--V	26.814	0	8.9	1.5	89.6	100
349 (EU)--V	27.024	0.5	7.8	4.2	87.5	100
350 (EU)--V	27.024	0.5	7.8	4.2	87.5	100
351 A1G)--V	27.4	0	4	3.6	92.3	100
352 (EU)--V	27.411	0	6.7	5.8	87.4	100
353 (EU)--V	27.411	0	6.7	5.8	87.4	100
354 (A1G)--V	27.756	0.2	6.2	6.5	87.2	100
355 (B2G)--V	28.099	0	6.6	4	89.5	100
356 (EU)--V	28.615	0	2.1	2.9	94.9	100
357 (EU)--V	28.615	0	2.1	2.9	94.9	100
358 (A2G)--V	28.842	0	0.9	0.2	99	100
359 (A2G)--V	29.599	0	2.7	2.6	94.7	100
360 (B1G)--V	29.649	0	1.7	16	82.3	100
361 (EU)--V	29.929	0.1	1.4	0.6	97.9	100
362 (EU)--V	29.929	0.1	1.4	0.6	97.9	100
363 (B2G)--V	30.029	0	0.7	4.7	94.5	100
364 (B1G)--V	30.268	0	5.5	11.1	83.4	100
365 (A1G)--V	30.531	1.1	6.7	3.6	88.5	100
366 (EU)--V	30.759	0.1	5.4	2.7	91.8	100
367 (EU)--V	30.759	0.1	5.4	2.7	91.8	100
368 (B2G)--V	31.15	0	1.5	1.9	96.6	100
369 (A1G)--V	31.732	5.3	3.6	0.3	90.7	100
370 (EU)--V	31.924	1.1	8.2	4.7	86.1	100
371 (EU)--V	31.924	1.1	8.2	4.7	86.1	100
372 (A2G)--V	32.167	0	1.6	13.9	84.4	100
373 (B2U)--V	32.179	0	8.2	8.7	83.2	100
374 (EG)--V	32.563	0.2	5.7	14.4	79.7	100
375 (EG)--V	32.563	0.2	5.7	14.4	79.7	100
376 B1G)--V	32.568	0.3	10.7	8.8	80.2	100
377 (EU)--V	33.149	0.2	3.2	9.8	86.8	100
378 (EU)--V	33.149	0.2	3.2	9.8	86.8	100
379 (A2U)--V	33.214	0.2	0.9	10.5	88.5	100
380 (B2G)--V	33.447	0	1.6	2	96.3	100
381 A1U)--V	34.024	0	20.1	18.5	61.4	100
382 (EG)--V	34.095	0	8.4	9.7	81.9	100
383 (EG)--V	34.095	0	8.4	9.7	81.9	100
384 (EU)--V	34.172	0.2	1.6	12.8	85.3	100
385 (EU)--V	34.172	0.2	1.6	12.8	85.3	100
386 B2U)--V	34.193	0	6	9.6	84.4	100
387 (A2G)--V	34.698	0	0.7	8.2	91.1	100
388 (B1G)--V	34.95	0	0.4	4.5	95.1	100
389 (B1U)--V	35.079	0	5.3	6.5	88.2	100
390 (EG)--V	35.172	0.2	5.4	6.9	87.5	100
391 (EG)--V	35.172	0.2	5.4	6.9	87.5	100
392 (A1U)--V	35.408	0	3.8	5.6	90.7	100
393 (A1G)--V	35.604	3.3	5.3	0.1	91.2	100
394 (EU)--V	35.8	0.1	4.3	0.5	95.1	100
395 (EU)--V	35.8	0.1	4.3	0.5	95.1	100
396 B1G)--V	35.822	0	5.8	0.3	93.9	100



397 (A2U)--V	35.884	4.1	26.4	17.6	51.9	100
398 (EG)--V	36.016	2.2	18.4	7.8	71.6	100
399 (EG)--V	36.016	2.2	18.4	7.8	71.6	100
400 (EU)--V	36.643	0.3	6.6	0.2	92.9	100
401 (EU)--V	36.643	0.3	6.6	0.2	92.9	100
402 (B2U)--V	37.653	0	28.3	0.7	71	100
403 (A2G)--V	37.926	0	3	18	79	100
404 (A1G)--V	37.948	0	0.4	0	99.6	100
405 (B2G)--V	38.134	0	0.1	0.4	99.6	100
406 (EU)--V	38.168	0.1	1	1.4	97.5	100
407 (EU)--V	38.168	0.1	1	1.4	97.5	100
408 (B1G)--V	38.245	0	0.1	1	98.8	100
409 (EG)--V	38.432	0.2	4.3	6.1	89.4	100
410 (EG)--V	38.432	0.2	4.3	6.1	89.4	100
411 A2U)--V	38.451	0.5	1.9	1.9	95.7	100
412 (B2U)--V	38.523	0	0.3	0.7	99.1	100
413 (EG)--V	38.757	0.5	12.9	12.5	74.2	100
414 (EG)--V	38.757	0.5	12.9	12.5	74.2	100
415 (A2U)--V	38.997	2.3	10.3	0.7	86.7	100
416 B1U)--V	39.332	0	18.7	24.5	56.8	100
417 (B2U)--V	39.35	0	2.1	0.7	97.1	100
418 (EG)--V	39.612	0.3	7.2	3.8	88.6	100
419 (EG)--V	39.612	0.3	7.2	3.8	88.6	100
420 (A1U)--V	39.657	0	0	0	100	100
421 (EU)--V	39.664	0	1.2	0.6	98.2	100
422 (EU)--V	39.664	0	1.2	0.6	98.2	100
423 (B1U)--V	39.712	0	3.5	5	91.5	100
424 (EG)--V	39.725	0.5	11.6	7.2	80.7	100
425 (EG)--V	39.725	0.5	11.6	7.2	80.7	100
426 A2G)--V	40.192	0	4.5	0	95.5	100
427 (A2U)--V	40.552	7.8	39	6	47.2	100
428 (A2G)--V	41.208	0	1.5	4	94.5	100
429 (B2G)--V	41.914	0	0.1	1.4	98.6	100
430 (EU)--V	42.067	0.2	3.9	0.1	95.8	100
431 (EU)--V	42.067	0.2	3.9	0.1	95.8	100
432 (A1G)--V	42.374	0.1	41.1	0.8	58.1	100
433 (EU)--V	42.584	0.9	14.2	2.8	82.2	100
434 (EU)--V	42.584	0.9	14.2	2.8	82.2	100
435 (A1G)--V	43.695	0.3	43.1	1.2	55.4	100
436 B1G)--V	44.084	0	32.9	2.6	64.5	100
437 (B2G)--V	45.149	0	0.2	20	79.8	100
438 (EU)--V	45.717	0.7	0.8	43.6	54.8	100
439 (EU)--V	45.717	0.7	0.8	43.6	54.8	100
440 (A1G)--V	45.979	1	0.7	53.9	44.3	100
441 B1G)--V	46.543	0	44.1	10.4	45.5	100
442 (EU)--V	46.874	0.2	36.5	4.3	59.1	100
443 (EU)--V	46.874	0.2	36.5	4.3	59.1	100
444 (B1U)--V	46.978	0	1.5	12.4	86.1	100
445 (A1G)--V	47.016	0.5	44.7	2.8	51.9	100
446 (EG)--V	47.294	0	2.5	10	87.5	100
447 (EG)--V	47.294	0	2.5	10	87.5	100

448 (A1U)--V	47.764	0	3.6	2.7	93.7	100
449 (B1G)--V	48.127	0	53.4	1.6	45	100
450 (EU)--V	48.59	0.1	22.6	2.5	74.7	100
451 (EU)--V	48.59	0.1	22.6	2.5	74.7	100
452 (B2G)--V	48.62	0	0.1	9.8	90.1	100
453 (A1G)--V	48.658	0.1	20.7	3.3	76	100
454 (EU)--V	48.904	0.1	0.7	23	76.2	100
455 (EU)--V	48.904	0.1	0.7	23	76.2	100
456 A2G)--V	49.061	0	0.6	0	99.4	100
457 (A2U)--V	49.123	0.5	10.5	25.1	64	100
458 (A1G)--V	49.418	0.6	18.8	41	39.6	100
459 (B1G)--V	49.896	0	31.2	5.2	63.6	100
460 (EU)--V	49.915	0.1	9.2	1.2	89.4	100
461 (EU)--V	49.915	0.1	9.2	1.2	89.4	100
462 (EG)--V	50.182	0.5	16	17.5	66	100
463 (EG)--V	50.182	0.5	16	17.5	66	100
464 (A2G)--V	50.357	0	0	0.1	99.9	100
465 (B2G)--V	50.883	0	0	1	99	100
466 (EU)--V	50.925	0	0.6	1.4	98	100
467 (EU)--V	50.925	0	0.6	1.4	98	100
468 (A1G)--V	51.017	0	10.7	37.6	51.6	100
469 (EU)--V	51.221	1.8	5.2	10.7	82.3	100
470 (EU)--V	51.221	1.8	5.2	10.7	82.3	100
471 B2U)--V	51.232	0	26.4	11.7	61.9	100
472 (B1G)--V	51.331	0	13.8	5.1	81	100
473 (B1G)--V	51.513	0	6.4	2.3	91.3	100
474 (EU)--V	51.733	5	12.1	6	76.9	100
475 (EU)--V	51.733	5	12.1	6	76.9	100
476 (EU)--V	52.176	10	27.5	1	61.5	100
477 (EU)--V	52.176	10	27.5	1	61.5	100
478 (A1G)--V	52.651	0.5	7.2	12.8	79.4	100
479 (A2G)--V	52.773	0	0.1	0.6	99.3	100
480 (B2G)--V	53.171	0	0.3	7.8	91.9	100
481 B2U)--V	53.449	0	26.6	14.2	59.2	100
482 (EU)--V	53.544	0	2.9	1.1	96	100
483 (EU)--V	53.544	0	2.9	1.1	96	100
484 (EU)--V	54.272	0.1	6.8	4.2	89	100
485 (EU)--V	54.272	0.1	6.8	4.2	89	100
486 A1G)--V	54.342	0	18	13.8	68.2	100
487 (EG)--V	54.651	1.7	28.5	16.8	53	100
488 (EG)--V	54.651	1.7	28.5	16.8	53	100
489 (B1G)--V	54.711	0	29.1	4.3	66.6	100
490 (A2G)--V	55.754	0	7.3	4.4	88.2	100
491 B1U)--V	55.822	0	2.4	29.1	68.5	100
492 (EG)--V	55.861	6.1	4.4	20	69.4	100
493 (EG)--V	55.861	6.1	4.4	20	69.4	100
494 (A1U)--V	55.863	0	24.9	11.3	63.8	100
495 (A2U)--V	55.927	0.4	4.9	20.7	74.1	100
496 B2G)--V	55.992	0	0.2	0.2	99.6	100
497 (EU)--V	56.274	0.1	0.8	1.1	98	100
498 (EU)--V	56.274	0.1	0.8	1.1	98	100

499 (A2G)--V	56.367	0	2.1	2.3	95.6	100
500 (EU)--V	56.595	0	2.4	4.9	92.6	100
501 (EU)--V	56.595	0	2.4	4.9	92.6	100
502 (B1G)--V	57.125	0	4.8	9.3	85.9	100
503 (B2G)--V	57.275	0	0.3	6.2	93.5	100
504 (EU)--V	57.509	0	0.7	3.4	95.8	100
505 (EU)--V	57.509	0	0.7	3.4	95.8	100
506 (EG)--V	57.542	59	14.1	0.9	26	100
507 (EG)--V	57.542	59	14.1	0.9	26	100
508 (A1G)--V	57.763	0.7	4.4	0.8	94.1	100
509 (B1U)--V	58.451	0	10.1	13.2	76.7	100
510 (EG)--V	58.458	12.9	9.6	5.2	72.3	100
511 (EG)--V	58.458	12.9	9.6	5.2	72.3	100
512 (A1U)--V	59.337	0	5.4	4.9	89.7	100
513 (B2U)--V	59.453	0	1	0	99	100
514 (A2G)--V	59.46	0	0.1	0.3	99.7	100
515 (EU)--V	59.627	0	3.9	6.7	89.3	100
516 (EU)--V	59.627	0	3.9	6.7	89.3	100
517 (EG)--V	60.006	0.1	8.8	0.1	90.9	100
518 (EG)--V	60.006	0.1	8.8	0.1	90.9	100
519 (B1U)--V	60.124	0	6.4	1.5	92.1	100
520 (EG)--V	60.286	1.1	1.4	6.3	91.2	100
521 (EG)--V	60.286	1.1	1.4	6.3	91.2	100
522 (A2U)--V	60.365	0.3	34.2	5.4	60.1	100
523 (A2U)--V	60.469	0.1	8	1.4	90.6	100
524 (A2G)--V	60.543	0	3.4	1.5	95.1	100
525 (B2G)--V	60.561	0	0.2	11.8	88	100
526 A1U)--V	60.601	0	0.3	4.8	95	100
527 (EU)--V	61.039	2	13.4	16.7	67.9	100
528 (EU)--V	61.039	2	13.4	16.7	67.9	100
529 (B1G)--V	61.239	0	36.2	16.6	47.2	100
530 (B2U)--V	61.49	0	2.4	1.2	96.4	100
531 (EG)--V	61.507	0	8.5	4.5	86.9	100
532 (EG)--V	61.507	0	8.5	4.5	86.9	100
533 (A1G)--V	62.25	0.1	1.1	17.8	81	100
534 (B2G)--V	62.412	5.4	7	1.7	85.9	100
535 (B1U)--V	63.298	0	18	1.7	80.3	100
536 (EU)--V	63.649	0.1	1.8	26.5	71.6	100
537 (EU)--V	63.649	0.1	1.8	26.5	71.6	100
538 (EG)--V	64.338	0.6	15.3	8.6	75.4	100
539 (EG)--V	64.338	0.6	15.3	8.6	75.4	100
540 (A2G)--V	64.361	0	0.1	0	99.9	100
541 (EU)--V	64.734	0	0.2	0.3	99.4	100
542 (EU)--V	64.734	0	0.2	0.3	99.4	100
543 (B2G)--V	64.862	0	2.6	25.9	71.5	100
544 (B1G)--V	65.086	0	1.9	0.1	98	100
545 (B2G)--V	65.496	0.3	2.7	1.9	95.1	100
546 A1G)--V	66.499	2.4	17.2	2.4	78	100
547 (A1U)--V	66.538	0	2.6	6.7	90.7	100
548 (A2U)--V	66.68	0.2	8.7	19.1	72	100
549 (EU)--V	66.874	0.2	8.8	10.6	80.4	100

550 (EU)--V	66.874	0.2	8.8	10.6	80.4	100
551 (EG)--V	67.754	0	7.5	10	82.5	100
552 (EG)--V	67.754	0	7.5	10	82.5	100
553 (A1U)--V	68.824	0	13.6	12.4	74	100
554 (B1U)--V	68.959	0	12.2	8.3	79.5	100
555 (B1G)--V	69.761	0.8	58.2	4.5	36.5	100
556 A1G)--V	69.959	2.9	17.8	36.2	43.1	100
557 (A2G)--V	70.378	0	0.8	0.3	98.9	100
558 (EG)--V	70.735	0.3	7.2	10.9	81.5	100
559 (EG)--V	70.735	0.3	7.2	10.9	81.5	100
560 (EU)--V	70.791	0	0.5	0.8	98.6	100
561 (EU)--V	70.791	0	0.5	0.8	98.6	100
562 (B2G)--V	70.8	0	0.3	0.1	99.5	100
563 (EU)--V	70.975	0	14.2	8.8	77	100
564 (EU)--V	70.975	0	14.2	8.8	77	100
565 (B1G)--V	71.202	0	0.6	3.5	95.9	100
566 (EU)--V	71.401	0.1	26.5	25.5	47.9	100
567 (EU)--V	71.401	0.1	26.5	25.5	47.9	100
568 (A1G)--V	71.405	3	11.6	24.1	61.3	100
569 (B1U)--V	71.584	0	0.2	4.2	95.7	100
570 (A2G)--V	71.629	0	2	1.6	96.4	100
571 (EU)--V	71.718	0	10.8	8.5	80.6	100
572 (EU)--V	71.718	0	10.8	8.5	80.6	100
573 (B1G)--V	71.869	0	26.7	4	69.3	100
574 (A1G)--V	72.178	4.4	8	1.4	86.2	100
575 (B2U)--V	72.676	0	16	30.8	53.3	100
576 A1U)--V	72.838	0	5.4	16.6	77.9	100
577 (B1G)--V	72.849	0.2	24.4	3.7	71.8	100
578 (EG)--V	72.882	0.2	9.9	22	67.9	100
579 (EG)--V	72.882	0.2	9.9	22	67.9	100
580 (EU)--V	72.886	0.1	40.7	13.1	46.1	100
581 (EU)--V	72.886	0.1	40.7	13.1	46.1	100
582 (A1G)--V	73.07	0.1	54.7	19.4	25.8	100
583 (B2G)--V	73.94	0	0.3	8.8	90.8	100
584 (B2G)--V	74.175	0.1	4.2	21	74.7	100
585 (EU)--V	74.667	0	1.9	6.4	91.7	100
586 (EU)--V	74.667	0	1.9	6.4	91.7	100
587 (B1G)--V	74.955	1.2	53.2	5	40.6	100
588 (A2G)--V	75.02	0	0.8	6.6	92.6	100
589 (B2G)--V	75.54	0	0.1	0.4	99.5	100
590 (EU)--V	76.253	0	2.6	4.8	92.6	100
591 (EU)--V	76.253	0	2.6	4.8	92.6	100
592 (EU)--V	77.814	0.1	7.3	4.6	88	100
593 (EU)--V	77.814	0.1	7.3	4.6	88	100
594 (A2G)--V	77.969	0	1.2	2.6	96.2	100
595 (A1G)--V	78.243	0.2	21.3	25.1	53.4	100
596 (EU)--V	78.329	0.4	6.6	5.8	87.3	100
597 (EU)--V	78.329	0.4	6.6	5.8	87.3	100
598 (B1G)--V	79.83	0.8	6.2	5.8	87.2	100
599 (B2G)--V	79.856	0	0.1	7.6	92.3	100
600 (A2G)--V	80.875	0	0.4	0	99.6	100

601 A1G)--V	81.306	0.4	4	4.7	90.9	100
602 (EU)--V	81.416	0.1	9.5	10.7	79.7	100
603 (EU)--V	81.416	0.1	9.5	10.7	79.7	100
604 (A2G)--V	82.117	0	14.7	4.4	81	100
605 (B2G)--V	83.317	0	2.3	2.6	95.1	100
606 (EU)--V	83.781	0	1.1	5	94	100
607 (EU)--V	83.781	0	1.1	5	94	100
608 (EU)--V	86.192	0.2	7.2	19.6	73	100
609 (EU)--V	86.192	0.2	7.2	19.6	73	100
610 (B1G)--V	87.449	0.8	5.1	25.5	68.6	100
611 A1G)--V	89.39	0.4	4.2	54.9	40.6	100
612 (B2G)--V	89.923	0	1	1.8	97.1	100
613 (EU)--V	91.089	0	1.5	3	95.4	100
614 (EU)--V	91.089	0	1.5	3	95.4	100
615 (A2G)--V	91.738	0	8	13.1	79	100
616 A2G)--V	91.943	0	1	0.7	98.3	100
617 (EU)--V	93.798	0	5.3	4.2	90.5	100
618 (EU)--V	93.798	0	5.3	4.2	90.5	100
619 (B2G)--V	94.476	0	3.8	2.9	93.3	100

### LSDA Exchange Correlation Functional

Orbital	Index	E, eV	Zn	NZn	Nmeso	Pc	Total	
	1 A1G)--O	-9388.36		100	0	0	0	100
	2 (A1G)--O	-1132.17		100	0	0	0	100
	3 (A2U)--O	-999.684		100	0	0	0	100
	4 (EU)--O	-999.506		100	0	0	0	100
	5 (EU)--O	-999.506		100	0	0	0	100
	6 (EU)--O	-378.426		0	99.8	0	0.1	100
	7 (EU)--O	-378.426		0	99.8	0	0.1	100
	8 (B1G)--O	-378.426		0	99.8	0	0.2	100
	9 (A1G)--O	-378.425		0	99.9	0	0.1	100
	10 (EU)--O	-378.072		0	0	99.7	0.3	100
	11 (EU)--O	-378.072		0	0	99.7	0.3	100
	12 (B2G)--O	-378.072		0	0	99.7	0.3	100
	13 (A1G)--O	-378.072		0	0	99.8	0.2	100
	14 (EU)--O	-268.771		0	0.1	0.1	99.8	100
	15 (EU)--O	-268.771		0	0.1	0.1	99.8	100
	16 B2G)--O	-268.771		0	0	0.3	99.7	100
	17 (A1G)--O	-268.77		0	0.1	0	99.9	100
	18 (A2G)--O	-268.769		0	0	0	100	100
	19 (EU)--O	-268.769		0	0	0	99.9	100
	20 (EU)--O	-268.769		0	0	0	99.9	100
	21 B1G)--O	-268.768		0	0.1	0	99.9	100
	22 (EU)--O	-267.008		0	0	0	100	100
	23 (EU)--O	-267.008		0	0	0	100	100
	24 (A1G)--O	-267.008		0	0	0	100	100



25 (B1G)--O	-267.008	0	0	0	100	100
26 A2G)--O	-267.005	0	0	0	100	100
27 (EU)--O	-267.005	0	0	0	100	100
28 (EU)--O	-267.005	0	0	0	100	100
29 (B2G)--O	-267.005	0	0	0	100	100
30 (A2G)--O	-266.95	0	0	0	100	100
31 (EU)--O	-266.95	0	0	0	100	100
32 (EU)--O	-266.95	0	0	0	100	100
33 (B2G)--O	-266.95	0	0	0	100	100
34 (B1G)--O	-266.949	0	0	0	100	100
35 (EU)--O	-266.949	0	0	0	100	100
36 (EU)--O	-266.949	0	0	0	100	100
37 (A1G)--O	-266.949	0	0	0	100	100
38 (B1G)--O	-266.934	0	0	0	100	100
39 (EU)--O	-266.934	0	0	0	100	100
40 (EU)--O	-266.934	0	0	0	100	100
41 A1G)--O	-266.934	0	0	0	100	100
42 (A2G)--O	-266.931	0	0	0	100	100
43 (EU)--O	-266.931	0	0	0	100	100
44 (EU)--O	-266.931	0	0	0	100	100
45 (B2G)--O	-266.931	0	0	0	100	100
46 A1G)--O	-124.845	100	0	0	0	100
47 (A2U)--O	-82.855	100	0	0	0	100
48 (EU)--O	-82.543	100	0	0	0	100
49 (EU)--O	-82.543	100	0	0	0	100
50 (A1G)--O	-25.6	0.5	40	24.5	35	100
51 (EU)--O	-25.232	0.2	39.3	23.7	36.8	100
52 (EU)--O	-25.232	0.2	39.3	23.7	36.8	100
53 (B1G)--O	-24.533	0.1	58.6	0.8	40.5	100
54 (B2G)--O	-23.932	0	2	68.7	29.3	100
55 (EU)--O	-22.903	0	17.2	49.8	32.9	100
56 (EU)--O	-22.903	0	17.2	49.8	32.9	100
57 (A1G)--O	-22.105	0.1	16.9	50.1	32.9	100
58 (A1G)--O	-21.614	0.4	19.9	6.5	73.2	100
59 (EU)--O	-21.59	0.1	13.9	1.1	84.9	100
60 (EU)--O	-21.59	0.1	13.9	1.1	84.9	100
61 B1G)--O	-21.575	0.1	12.6	0	87.3	100
62 (A2G)--O	-19.56	0	3.3	7.7	89	100
63 (A1G)--O	-19.235	0.8	12.7	0.3	86.2	100
64 (EU)--O	-19.193	0.1	14.4	4.4	81.1	100
65 (EU)--O	-19.193	0.1	14.4	4.4	81.1	100
66 (EU)--O	-19.072	0	3.7	1.5	94.7	100
67 (EU)--O	-19.072	0	3.7	1.5	94.7	100
68 (B1G)--O	-19.066	0.4	19.1	0.8	79.7	100
69 (B2G)--O	-18.978	0	0	1.7	98.2	100
70 (A2G)--O	-18.213	0	5.7	8.4	85.9	100
71 (EU)--O	-17.609	0	6.8	18.3	74.8	100
72 (EU)--O	-17.609	0	6.8	18.3	74.8	100

73(B1G)--O	-16.304	0.5	7.9	24.1	67.4	100
74(A1G)--O	-16.146	2.6	11.9	0.7	84.8	100
75(EU)--O	-15.964	0.3	11.4	0.6	87.8	100
76(EU)--O	-15.964	0.3	11.4	0.6	87.8	100
77(B2G)--O	-15.785	0.1	3.5	14.1	82.3	100
78(B1G)--O	-15.766	1	9.2	6.6	83.3	100
79(B2G)--O	-15.156	1.6	30.2	22.2	45.9	100
80(EU)--O	-15.115	0.1	7.5	3.1	89.4	100
81(EU)--O	-15.115	0.1	7.5	3.1	89.4	100
82(A2G)--O	-14.855	0	7	1.4	91.6	100
83(A1G)--O	-14.18	3.2	7.7	1.3	87.7	100
84(EU)--O	-14.052	0	19.9	17	63.1	100
85(EU)--O	-14.052	0	19.9	17	63.1	100
86(EU)--O	-13.686	0.4	10.3	15.3	74.1	100
87(EU)--O	-13.686	0.4	10.3	15.3	74.1	100
88(B1G)--O	-13.615	5.9	12.8	5.1	76.2	100
89(A2G)--O	-12.937	0	21.1	14.1	64.8	100
90(B2G)--O	-12.685	0.9	1.6	1.5	96	100
91 A1G)--O	-12.447	21.9	20.8	2.1	55.1	100
92(B1G)--O	-12.224	34.7	18.7	0.3	46.2	100
93(EU)--O	-12.207	0	3.1	4	93	100
94(EU)--O	-12.207	0	3.1	4	93	100
95(A2U)--O	-12.028	0.5	25.2	17.8	56.6	100
96(EU)--O	-11.864	0.7	13	1.8	84.5	100
97(EU)--O	-11.864	0.7	13	1.8	84.5	100
98(EG)--O	-11.735	18.1	24.8	12.2	44.9	100
99(EG)--O	-11.735	18.1	24.8	12.2	44.9	100
100(A2G)--O	-11.671	0	1	6.9	92.1	100
101 A1G)--O	-11.402	9.4	9.7	6.2	74.7	100
102(B1G)--O	-11.356	21	10.8	1.9	66.3	100
103(EU)--O	-11.152	0.1	1.6	1.4	96.9	100
104(EU)--O	-11.152	0.1	1.6	1.4	96.9	100
105(B2G)--O	-11.133	0.2	0.1	0.6	99	100
106 A1G)--O	-11.01	40.5	4	2.3	53.2	100
107(A2G)--O	-10.907	0	0.6	3.3	96.1	100
108(B2U)--O	-10.9	0	26.6	0	73.4	100
109(EU)--O	-10.843	0.4	5.6	4.1	89.9	100
110(EU)--O	-10.843	0.4	5.6	4.1	89.9	100
111(EG)--O	-10.659	88.3	1.2	1.9	8.5	100
112(EG)--O	-10.659	88.3	1.2	1.9	8.5	100
113(B2G)--O	-10.595	49.3	6.6	0.9	43.2	100
114(B1G)--O	-10.456	15.3	1	3.2	80.5	100
115(B1U)--O	-10.045	0	0	50.4	49.6	100
116 A1G)--O	-10.027	62.9	11.1	2.6	23.3	100
117(EG)--O	-9.497	2.2	1.7	15.4	80.7	100
118(EG)--O	-9.497	2.2	1.7	15.4	80.7	100
119(A2U)--O	-9.471	0.4	7	3.9	88.7	100
120(B2G)--O	-9.38	0.9	0.1	1.4	97.6	100

121 (EU)--O	-9.315	0.1	1.7	1.8	96.5	100
122 (EU)--O	-9.315	0.1	1.7	1.8	96.5	100
123 (A2G)--O	-9.141	0	1.7	0.9	97.4	100
124 (B2U)--O	-9.09	0	25.3	0	74.7	100
125 (EU)--O	-9.036	6.2	37.9	2.8	53.1	100
126 (EU)--O	-9.036	6.2	37.9	2.8	53.1	100
127 (A1G)--O	-8.953	0	2.2	3	94.8	100
128 (EU)--O	-8.657	1.9	10.4	5.6	82.1	100
129 (EU)--O	-8.657	1.9	10.4	5.6	82.1	100
130 (B1G)--O	-8.618	1.4	0.6	2.7	95.3	100
131 (EG)--O	-8.438	3.3	19.6	19.9	57.2	100
132 (EG)--O	-8.438	3.3	19.6	19.9	57.2	100
133 (A1G)--O	-7.539	0.1	19.8	51.5	28.6	100
134 (A1U)--O	-7.43	0	0	0	99.9	100
135 (A2U)--O	-7.009	3.4	48.7	27.9	20.1	100
136 B1U)--O	-6.925	0	0	5.2	94.8	100
137 (EG)--O	-6.906	0	0.4	9.9	89.6	100
138 (EG)--O	-6.906	0	0.4	9.9	89.6	100
139 (EU)--O	-6.89	0.2	17.9	48.3	33.5	100
140 (EU)--O	-6.89	0.2	17.9	48.3	33.5	100
141 A2U)--O	-6.824	0	2.2	33	64.7	100
142 (EG)--O	-6.696	2.1	28.4	1.6	67.9	100
143 (EG)--O	-6.696	2.1	28.4	1.6	67.9	100
144 (B2U)--O	-6.683	0	25.9	0	74.1	100
145 (B2G)--O	-6.426	0.7	11.7	59.2	28.5	100
146 B1G)--O	-5.958	24.1	48.4	0.8	26.7	100
147 (A1U)--O	-5.379	0	0.1	0.1	99.8	100
148 (EG)--V	-3.923	0.4	13.3	19.9	66.3	100
149 (EG)--V	-3.923	0.4	13.3	19.9	66.3	100
150 (B1U)--V	-2.496	0	0	25.4	74.5	100
151 B2U)--V	-2.275	0	19.8	0	80.2	100
152 (A2U)--V	-2.153	6.4	1.1	5.7	86.8	100
153 (EG)--V	-2.004	0.1	5.7	3.7	90.5	100
154 (EG)--V	-2.004	0.1	5.7	3.7	90.5	100
155 (A1U)--V	-0.831	0	0	0	100	100
156 (EG)--V	-0.776	0	1.7	0.9	97.3	100
157 (EG)--V	-0.776	0	1.7	0.9	97.3	100
158 (A2U)--V	-0.509	59.3	7.3	2.9	30.5	100
159 (A1G)--V	-0.248	68.6	19.6	0.4	11.4	100
160 (B2U)--V	-0.23	0	19.4	0.1	80.6	100
161 B1U)--V	-0.032	0	0.1	18.5	81.5	100
162 (EG)--V	1.247	0.1	14.5	16	69.4	100
163 (EG)--V	1.247	0.1	14.5	16	69.4	100
164 (A1G)--V	1.34	0.2	0.1	2	97.7	100
165 (EU)--V	1.379	14.2	2.6	1.8	81.4	100
166 (EU)--V	1.379	14.2	2.6	1.8	81.4	100
167 (B1G)--V	1.528	0	0	0.1	99.9	100
168 (EU)--V	1.636	52.3	8.1	1.9	37.7	100

169 (EU)--V	1.636	52.3	8.1	1.9	37.7	100
170 (A2U)--V	1.989	25.5	18.3	16.7	39.5	100
171 B2G)--V	2.334	0	1.1	0.2	98.7	100
172 (A1G)--V	2.524	38.4	0.5	11.9	49.2	100
173 (EU)--V	2.533	0	1.3	0.2	98.5	100
174 (EU)--V	2.533	0	1.3	0.2	98.5	100
175 (A2G)--V	2.778	0	0.7	0	99.2	100
176 A1U)--V	2.891	0	0	0	100	100
177 (EG)--V	3.063	0	0.9	4	95.1	100
178 (EG)--V	3.063	0	0.9	4	95.1	100
179 (B1U)--V	3.081	0	0	4.6	95.4	100
180 (EU)--V	3.229	1.5	0.2	3.9	94.4	100
181 (EU)--V	3.229	1.5	0.2	3.9	94.4	100
182 (B2G)--V	3.235	0	0.2	7.1	92.7	100
183 (A1G)--V	3.451	27.9	0.9	0.2	71.1	100
184 (B1G)--V	3.563	0	7.3	0.4	92.3	100
185 (EU)--V	3.581	1.8	3	0.4	94.8	100
186 (EU)--V	3.581	1.8	3	0.4	94.8	100
187 (A2G)--V	3.824	0	0.2	0.1	99.8	100
188 (B2G)--V	4.194	0.1	3	9.1	87.8	100
189 (EU)--V	4.228	5	7.6	3.1	84.4	100
190 (EU)--V	4.228	5	7.6	3.1	84.4	100
191 A1G)--V	4.395	0.1	0.9	1.5	97.5	100
192 (B1G)--V	4.424	0	25.4	3.4	71.2	100
193 (EU)--V	4.95	0.1	0.7	1.2	97.9	100
194 (EU)--V	4.95	0.1	0.7	1.2	97.9	100
195 (A2U)--V	4.965	90	2.4	0.8	6.8	100
196 A2G)--V	5.027	0	5.9	0.6	93.5	100
197 (EU)--V	5.309	1.2	0.3	6.4	92.1	100
198 (EU)--V	5.309	1.2	0.3	6.4	92.1	100
199 (B2G)--V	5.391	0	0.3	11.2	88.5	100
200 (B1G)--V	5.61	0	3	0	97	100
201 A2G)--V	5.656	0	0.2	0	99.8	100
202 (A1G)--V	5.95	8.9	9.9	19.4	61.8	100
203 (EU)--V	5.96	1.7	6	2.4	89.9	100
204 (EU)--V	5.96	1.7	6	2.4	89.9	100
205 (EU)--V	6.286	0.9	6.3	2.8	90	100
206 (EU)--V	6.286	0.9	6.3	2.8	90	100
207 (A1G)--V	6.437	5.8	0.6	3.7	89.9	100
208 (B2G)--V	7.025	0	0.7	3.5	95.8	100
209 (B1G)--V	7.032	0	0.4	0.1	99.5	100
210 (EU)--V	7.344	0.3	2.9	13.8	83	100
211 (EU)--V	7.344	0.3	2.9	13.8	83	100
212 (EU)--V	7.565	2.2	3.8	0.4	93.7	100
213 (EU)--V	7.565	2.2	3.8	0.4	93.7	100
214 (A1G)--V	7.576	0.2	1.8	2.7	95.4	100
215 (B2G)--V	7.792	0	4.9	24.8	70.3	100
216 B1G)--V	8.127	0	4.2	0.1	95.7	100

217 (B2G)--V	8.308	0	0.8	13.4	85.7	100
218 (A2G)--V	8.635	0	7.2	9	83.8	100
219 (EU)--V	8.701	2.7	3.8	17.4	76	100
220 (EU)--V	8.701	2.7	3.8	17.4	76	100
221 A1G)--V	8.765	1	16.2	12.8	70	100
222 (EU)--V	9.518	3	11.2	7.1	78.7	100
223 (EU)--V	9.518	3	11.2	7.1	78.7	100
224 (A2G)--V	9.589	0	0	0.6	99.4	100
225 (EU)--V	9.712	0.8	1.5	3.9	93.7	100
226 (EU)--V	9.712	0.8	1.5	3.9	93.7	100
227 (B1G)--V	9.748	0	19.1	7.7	73.2	100
228 (EU)--V	11.37	2.4	4.5	4.3	88.8	100
229 (EU)--V	11.37	2.4	4.5	4.3	88.8	100
230 (A2G)--V	11.533	0	0.3	7.2	92.5	100
231 (EG)--V	11.731	0	1.6	1.4	97	100
232 (EG)--V	11.731	0	1.6	1.4	97	100
233 (B2G)--V	11.903	0	0.4	0.1	99.4	100
234 (B2U)--V	11.952	0	0.4	0	99.6	100
235 (A2U)--V	12.07	4.1	0.1	0.7	95.1	100
236 (EU)--V	12.59	0.1	0.6	3.9	95.3	100
237 (EU)--V	12.59	0.1	0.6	3.9	95.3	100
238 (EG)--V	12.592	0	2.3	1.6	96.1	100
239 (EG)--V	12.592	0	2.3	1.6	96.1	100
240 (A1G)--V	12.763	0.7	2.8	0.9	95.6	100
241 B1U)--V	12.887	0	0	4.6	95.4	100
242 (A2G)--V	12.888	0	1.1	3.2	95.7	100
243 (B2G)--V	13.053	0	0.5	2.8	96.7	100
244 (B1G)--V	13.125	0	33.8	5.2	61	100
245 (EU)--V	13.249	0.3	0.3	0.2	99.2	100
246 (EU)--V	13.249	0.3	0.3	0.2	99.2	100
247 (B1G)--V	13.393	0	2.5	2.8	94.7	100
248 (B2U)--V	13.422	0	1.3	0.1	98.6	100
249 (EU)--V	13.462	0	0.4	0.5	99	100
250 (EU)--V	13.462	0	0.4	0.5	99	100
251 A2U)--V	13.559	11.1	1.4	1.4	86.1	100
252 (B2G)--V	13.603	0	0.6	1.4	98	100
253 (EG)--V	13.737	0	0.5	1.8	97.7	100
254 (EG)--V	13.737	0	0.5	1.8	97.7	100
255 (A2G)--V	13.775	0	0.2	0.6	99.2	100
256 A1G)--V	13.815	1.8	2.3	17.6	78.3	100
257 (A1U)--V	13.896	0	0	0	100	100
258 (EU)--V	13.987	0.1	1.3	2.3	96.3	100
259 (EU)--V	13.987	0.1	1.3	2.3	96.3	100
260 (B1G)--V	14.027	0	25.1	0.9	74	100
261 A1G)--V	14.426	1.1	0.2	13.1	85.7	100
262 (EU)--V	14.516	0.3	15.5	16.5	67.6	100
263 (EU)--V	14.516	0.3	15.5	16.5	67.6	100
264 (A2G)--V	14.682	0	0.9	2	97.1	100

265 (B1U)--V	14.69	0	0	1	99	100
266 B2G)--V	14.789	0	1	13.9	85.1	100
267 (A1G)--V	14.82	0.8	23.2	9.5	66.5	100
268 (EU)--V	14.839	0.1	0.4	0.9	98.6	100
269 (EU)--V	14.839	0.1	0.4	0.9	98.6	100
270 (B1G)--V	14.853	0	2	0.6	97.4	100
271 (EG)--V	14.885	0	4	0.5	95.5	100
272 (EG)--V	14.885	0	4	0.5	95.5	100
273 (A1G)--V	15.016	0.3	17.7	15.4	66.5	100
274 (EU)--V	15.079	1.7	20.6	9.6	68.2	100
275 (EU)--V	15.079	1.7	20.6	9.6	68.2	100
276 A2G)--V	15.134	0	0.8	2.8	96.4	100
277 (EU)--V	15.407	1.6	4.2	1.7	92.5	100
278 (EU)--V	15.407	1.6	4.2	1.7	92.5	100
279 (EU)--V	15.425	1.1	1.5	13.6	83.8	100
280 (EU)--V	15.425	1.1	1.5	13.6	83.8	100
281 (EG)--V	15.553	0	1.3	3.8	95	100
282 (EG)--V	15.553	0	1.3	3.8	95	100
283 (B2G)--V	15.585	0	0.7	13.2	86.1	100
284 (A2U)--V	15.606	3.1	1.2	1.3	94.3	100
285 (B2U)--V	15.698	0	1.8	0	98.2	100
286 A1U)--V	15.775	0	0	0	100	100
287 (B1G)--V	15.803	0.1	14.6	7.4	78	100
288 (B1U)--V	16.459	0	0	2.4	97.6	100
289 (EG)--V	16.575	0	0.6	0.3	99.1	100
290 (EG)--V	16.575	0	0.6	0.3	99.1	100
291 A2U)--V	16.746	0.8	0.4	4.4	94.5	100
292 (A1G)--V	16.806	6	24	3.5	66.5	100
293 (B2U)--V	18.032	0	1.1	0	98.9	100
294 (EG)--V	18.083	0	1.8	1.9	96.3	100
295 (EG)--V	18.083	0	1.8	1.9	96.3	100
296 A1U)--V	18.297	0	0	0	100	100
297 (EU)--V	18.385	5.8	15.6	7.1	71.5	100
298 (EU)--V	18.385	5.8	15.6	7.1	71.5	100
299 (B1U)--V	18.836	0	0	3.4	96.6	100
300 (EG)--V	19.211	0.3	36.5	6.7	56.5	100
301 (EG)--V	19.211	0.3	36.5	6.7	56.5	100
302 (B2G)--V	19.508	0	0.1	3.3	96.7	100
303 (EU)--V	19.752	0.1	1	1.5	97.5	100
304 (EU)--V	19.752	0.1	1	1.5	97.5	100
305 (A1G)--V	19.954	0.1	0.3	0.9	98.8	100
306 A2U)--V	19.977	1.3	12.4	54.6	31.7	100
307 (B2G)--V	20.167	0	3.5	3	93.5	100
308 (EG)--V	20.406	0	1.6	0.4	98	100
309 (EG)--V	20.406	0	1.6	0.4	98	100
310 (A2G)--V	20.481	0	0.4	0.6	99.1	100
311 (EU)--V	20.613	0.1	0.1	1.2	98.7	100
312 (EU)--V	20.613	0.1	0.1	1.2	98.7	100

313 (A2G)--V	20.99	0	1.5	1.7	96.8	100
314 (B2G)--V	21.1	0	7.7	5.9	86.4	100
315 (EU)--V	21.101	0	0.9	0.5	98.5	100
316 (EU)--V	21.101	0	0.9	0.5	98.5	100
317 (B1G)--V	21.153	0	1.2	0.6	98.2	100
318 (B2G)--V	21.574	0	0.9	5.6	93.5	100
319 (A1G)--V	21.635	0.4	9	7.1	83.6	100
320 (EU)--V	21.682	0.1	1.9	3.4	94.6	100
321 (EU)--V	21.682	0.1	1.9	3.4	94.6	100
322 (B2U)--V	21.744	0	67.7	0	32.3	100
323 (A2G)--V	21.899	0	0.6	9.3	90	100
324 (A1U)--V	21.985	0	0	0	100	100
325 (EU)--V	22.327	0.1	0.9	3.5	95.5	100
326 (EU)--V	22.327	0.1	0.9	3.5	95.5	100
327 (B1G)--V	22.35	0	0.2	0.2	99.5	100
328 (A1G)--V	22.399	3	3.6	29.6	63.7	100
329 (EG)--V	22.567	0.1	14.3	41.1	44.5	100
330 (EG)--V	22.567	0.1	14.3	41.1	44.5	100
331 B1U)--V	22.605	0	0	63.3	36.7	100
332 (B1G)--V	22.931	0	20.6	10	69.3	100
333 (EU)--V	22.968	0.4	3.7	8.8	87.1	100
334 (EU)--V	22.968	0.4	3.7	8.8	87.1	100
335 (A1G)--V	23.094	0.7	8.9	5	85.4	100
336 (EU)--V	23.527	0.3	8.5	4.6	86.6	100
337 (EU)--V	23.527	0.3	8.5	4.6	86.6	100
338 (A2G)--V	23.698	0	0	0	100	100
339 (B1G)--V	23.731	0	0.3	0.4	99.3	100
340 (EU)--V	24.144	0.3	0.2	3.4	96.1	100
341 (EU)--V	24.144	0.3	0.2	3.4	96.1	100
342 (A2G)--V	24.611	0	0	1.7	98.2	100
343 (B2G)--V	24.613	0	0	0.5	99.5	100
344 (A2U)--V	24.644	4.6	42.4	16.1	37	100
345 (EU)--V	24.764	0	0.7	2.4	96.9	100
346 (EU)--V	24.764	0	0.7	2.4	96.9	100
347 (B2G)--V	25.25	0	1.4	2.6	96	100
348 (B1G)--V	25.463	0	8.9	1.4	89.7	100
349 (EU)--V	25.671	0.6	7.8	4.2	87.5	100
350 (EU)--V	25.671	0.6	7.8	4.2	87.5	100
351 A1G)--V	26.047	0	4	3.6	92.4	100
352 (EU)--V	26.063	0	6.7	5.8	87.4	100
353 (EU)--V	26.063	0	6.7	5.8	87.4	100
354 (A1G)--V	26.381	0.2	6.2	6.5	87.2	100
355 (B2G)--V	26.75	0	6.6	3.9	89.5	100
356 (EU)--V	27.25	0	2.1	2.9	95	100
357 (EU)--V	27.25	0	2.1	2.9	95	100
358 (A2G)--V	27.474	0	0.9	0.1	99	100
359 (A2G)--V	28.227	0	2.6	2.5	94.9	100
360 (B1G)--V	28.283	0	1.6	15.8	82.5	100

361 (EU)--V	28.553	0.1	1.4	0.6	97.9	100
362 (EU)--V	28.553	0.1	1.4	0.6	97.9	100
363 (B2G)--V	28.654	0	0.7	4.8	94.5	100
364 (B1G)--V	28.903	0	5.5	11.3	83.1	100
365 (A1G)--V	29.169	1.1	6.7	3.6	88.6	100
366 (EU)--V	29.39	0.1	5.3	2.7	91.8	100
367 (EU)--V	29.39	0.1	5.3	2.7	91.8	100
368 (B2G)--V	29.773	0	1.5	1.8	96.7	100
369 (A1G)--V	30.346	5.4	3.7	0.3	90.6	100
370 (EU)--V	30.555	1.1	8.1	4.6	86.2	100
371 (EU)--V	30.555	1.1	8.1	4.6	86.2	100
372 (B2U)--V	30.708	0	8.2	8.7	83.1	100
373 (A2G)--V	30.779	0	1.7	13.9	84.5	100
374 (EG)--V	31.094	0.2	5.7	14.5	79.5	100
375 (EG)--V	31.094	0.2	5.7	14.5	79.5	100
376 B1G)--V	31.169	0.3	10.4	9	80.3	100
377 (A2U)--V	31.746	0.2	0.9	10.6	88.3	100
378 (EU)--V	31.792	0.2	3.2	9.6	87	100
379 (EU)--V	31.792	0.2	3.2	9.6	87	100
380 (B2G)--V	32.069	0	1.6	2	96.3	100
381 A1U)--V	32.548	0	20	18.5	61.6	100
382 (EG)--V	32.623	0	8.4	9.7	81.9	100
383 (EG)--V	32.623	0	8.4	9.7	81.9	100
384 (B2U)--V	32.721	0	6	9.6	84.3	100
385 (EU)--V	32.795	0.2	1.7	13	85.1	100
386 (EU)--V	32.795	0.2	1.7	13	85.1	100
387 (A2G)--V	33.343	0	0.7	8.1	91.2	100
388 (B1G)--V	33.546	0	0.4	4.6	95	100
389 (B1U)--V	33.612	0	5.3	6.5	88.3	100
390 (EG)--V	33.702	0.2	5.3	6.9	87.5	100
391 (EG)--V	33.702	0.2	5.3	6.9	87.5	100
392 (A1U)--V	33.935	0	3.8	5.5	90.7	100
393 (A1G)--V	34.223	3.3	5.3	0.1	91.2	100
394 (EU)--V	34.42	0.1	4.4	0.5	95	100
395 (EU)--V	34.42	0.1	4.4	0.5	95	100
396 A2U)--V	34.43	4.2	26.5	17.6	51.7	100
397 (B1G)--V	34.448	0	5.8	0.3	93.9	100
398 (EG)--V	34.552	2.2	18.4	7.8	71.6	100
399 (EG)--V	34.552	2.2	18.4	7.8	71.6	100
400 (EU)--V	35.266	0.3	6.7	0.2	92.8	100
401 (EU)--V	35.266	0.3	6.7	0.2	92.8	100
402 (B2U)--V	36.19	0	28.3	0.7	71	100
403 (A2G)--V	36.559	0	3	18	79	100
404 (A1G)--V	36.569	0	0.4	0	99.6	100
405 (B2G)--V	36.757	0	0.1	0.4	99.6	100
406 (EU)--V	36.789	0.1	1	1.4	97.5	100
407 (EU)--V	36.789	0.1	1	1.4	97.5	100
408 (B1G)--V	36.866	0	0.1	1	98.8	100



409(EG)--V	36.964	0.2	4.3	6.2	89.2	100
410(EG)--V	36.964	0.2	4.3	6.2	89.2	100
411 A2U)--V	36.984	0.5	1.9	1.9	95.6	100
412 (B2U)--V	37.055	0	0.3	0.7	99.1	100
413 (EG)--V	37.289	0.5	12.9	12.5	74.1	100
414 (EG)--V	37.289	0.5	12.9	12.5	74.1	100
415 (A2U)--V	37.531	2.4	10.3	0.7	86.6	100
416 B1U)--V	37.858	0	18.8	24.7	56.5	100
417 (B2U)--V	37.881	0	2.1	0.7	97.2	100
418 (EG)--V	38.143	0.3	7.4	3.9	88.3	100
419 (EG)--V	38.143	0.3	7.4	3.9	88.3	100
420 (A1U)--V	38.189	0	0	0	100	100
421 B1U)--V	38.242	0	3.4	4.9	91.8	100
422 (EG)--V	38.255	0.5	11.3	7	81.1	100
423 (EG)--V	38.255	0.5	11.3	7	81.1	100
424 (EU)--V	38.284	0	1.2	0.6	98.2	100
425 (EU)--V	38.284	0	1.2	0.6	98.2	100
426 A2G)--V	38.813	0	4.4	0	95.5	100
427 (A2U)--V	39.08	7.8	39	6	47.1	100
428 (A2G)--V	39.824	0	1.5	3.9	94.5	100
429 (B2G)--V	40.512	0	0.1	1.4	98.6	100
430 (EU)--V	40.651	0.2	3.7	0.1	96	100
431 (EU)--V	40.651	0.2	3.7	0.1	96	100
432 (A1G)--V	40.968	0.1	40.8	0.8	58.4	100
433 (EU)--V	41.192	0.9	14.6	2.8	81.7	100
434 (EU)--V	41.192	0.9	14.6	2.8	81.7	100
435 (A1G)--V	42.25	0.3	43.2	1.2	55.3	100
436 B1G)--V	42.672	0	32.6	2.6	64.9	100
437 (B2G)--V	43.749	0	0.2	19.8	80	100
438 (EU)--V	44.291	0.7	0.9	43.5	54.9	100
439 (EU)--V	44.291	0.7	0.9	43.5	54.9	100
440 (A1G)--V	44.562	1.1	0.7	53.5	44.7	100
441 B1G)--V	45.11	0	44	10.4	45.6	100
442 (EU)--V	45.445	0.2	36.7	4.3	58.8	100
443 (EU)--V	45.445	0.2	36.7	4.3	58.8	100
444 (B1U)--V	45.532	0	1.5	12.4	86.2	100
445 (A1G)--V	45.59	0.5	44.8	2.9	51.8	100
446 (EG)--V	45.849	0	2.5	10	87.6	100
447 (EG)--V	45.849	0	2.5	10	87.6	100
448 (A1U)--V	46.316	0	3.6	2.7	93.7	100
449 (B1G)--V	46.689	0	53.4	1.5	45	100
450 (EU)--V	47.157	0.1	22.7	2.5	74.7	100
451 (EU)--V	47.157	0.1	22.7	2.5	74.7	100
452 (B2G)--V	47.206	0	0.1	10.4	89.5	100
453 (A1G)--V	47.221	0.1	20.6	3.6	75.7	100
454 (EU)--V	47.488	0.1	0.6	23.6	75.7	100
455 (EU)--V	47.488	0.1	0.6	23.6	75.7	100
456 A2G)--V	47.653	0	0.6	0	99.4	100

457 (A2U)--V	47.672	0.5	10.5	25.1	64	100
458 (A1G)--V	47.997	0.6	18.8	41	39.6	100
459 (B1G)--V	48.473	0	31.2	5.2	63.6	100
460 (EU)--V	48.491	0.1	9.8	1.3	88.8	100
461 (EU)--V	48.491	0.1	9.8	1.3	88.8	100
462 (EG)--V	48.728	0.5	16	17.5	66.1	100
463 (EG)--V	48.728	0.5	16	17.5	66.1	100
464 (A2G)--V	48.943	0	0	0.1	99.9	100
465 (B2G)--V	49.503	0	0	1	99	100
466 (EU)--V	49.539	0.1	0.6	1.4	98	100
467 (EU)--V	49.539	0.1	0.6	1.4	98	100
468 (A1G)--V	49.575	0	10.7	37.8	51.4	100
469 (B2U)--V	49.773	0	26.4	11.7	61.9	100
470 (EU)--V	49.793	1.6	4.7	10.1	83.6	100
471 (EU)--V	49.793	1.6	4.7	10.1	83.6	100
472 (B1G)--V	49.905	0	14.1	5.2	80.7	100
473 (B1G)--V	50.066	0	6.5	2.3	91.2	100
474 (EU)--V	50.295	4.5	11.8	6.2	77.5	100
475 (EU)--V	50.295	4.5	11.8	6.2	77.5	100
476 (EU)--V	50.764	10.5	28	0.9	60.6	100
477 (EU)--V	50.764	10.5	28	0.9	60.6	100
478 (A1G)--V	51.214	0.5	7.3	12.8	79.4	100
479 (A2G)--V	51.369	0	0.1	0.6	99.3	100
480 (B2G)--V	51.734	0	0.3	7.8	91.9	100
481 B2U)--V	51.986	0	26.6	14.2	59.2	100
482 (EU)--V	52.116	0	2.9	1.1	96	100
483 (EU)--V	52.116	0	2.9	1.1	96	100
484 (EU)--V	52.841	0.1	6.6	4.1	89.3	100
485 (EU)--V	52.841	0.1	6.6	4.1	89.3	100
486 A1G)--V	52.905	0	18	13.8	68.1	100
487 (EG)--V	53.189	1.6	28.6	16.9	53	100
488 (EG)--V	53.189	1.6	28.6	16.9	53	100
489 (B1G)--V	53.278	0	29.1	4.3	66.6	100
490 (A2G)--V	54.33	0	7.5	4.5	88	100
491 B1U)--V	54.361	0	2.4	29.2	68.4	100
492 (A1U)--V	54.398	0	24.9	11.3	63.7	100
493 (EG)--V	54.403	5.9	4.5	20.1	69.6	100
494 (EG)--V	54.403	5.9	4.5	20.1	69.6	100
495 (A2U)--V	54.467	0.4	4.9	20.7	74	100
496 B2G)--V	54.557	0	0.2	0.2	99.6	100
497 (EU)--V	54.837	0.1	0.8	1.1	98	100
498 (EU)--V	54.837	0.1	0.8	1.1	98	100
499 (A2G)--V	54.946	0	2.2	2.4	95.4	100
500 (EU)--V	55.168	0	2.4	4.8	92.7	100
501 (EU)--V	55.168	0	2.4	4.8	92.7	100
502 (B1G)--V	55.689	0	4.8	9.3	85.9	100
503 (B2G)--V	55.849	0	0.3	6.1	93.6	100
504 (EU)--V	56.075	0	0.7	3.4	95.8	100

505 (EU)--V	56.075	0	0.7	3.4	95.8	100
506 (EG)--V	56.114	58.3	14.2	0.9	26.6	100
507 (EG)--V	56.114	58.3	14.2	0.9	26.6	100
508 (A1G)--V	56.325	0.7	4.4	0.8	94.1	100
509 (B1U)--V	56.984	0	10.2	13.1	76.7	100
510 (EG)--V	56.998	13.8	9.6	5.2	71.4	100
511 (EG)--V	56.998	13.8	9.6	5.2	71.4	100
512 (A1U)--V	57.877	0	5.4	4.9	89.7	100
513 (B2U)--V	57.989	0	1	0	99	100
514 (A2G)--V	58.026	0	0.1	0.3	99.7	100
515 (EU)--V	58.195	0	3.9	6.7	89.3	100
516 (EU)--V	58.195	0	3.9	6.7	89.3	100
517 (EG)--V	58.542	0.1	8.8	0.1	91	100
518 (EG)--V	58.542	0.1	8.8	0.1	91	100
519 (B1U)--V	58.663	0	6.3	1.5	92.1	100
520 (EG)--V	58.822	1.2	1.4	6.2	91.2	100
521 (EG)--V	58.822	1.2	1.4	6.2	91.2	100
522 (A2U)--V	58.898	0.3	34.6	5.4	59.8	100
523 (A2U)--V	59.002	0.1	7.5	1.4	90.9	100
524 (A2G)--V	59.1	0	3.3	1.5	95.2	100
525 (B2G)--V	59.127	0	0.2	11.8	88	100
526 A1U)--V	59.134	0	0.3	4.8	95	100
527 (EU)--V	59.603	2.1	13.3	16.6	68	100
528 (EU)--V	59.603	2.1	13.3	16.6	68	100
529 (B1G)--V	59.819	0	36.2	16.6	47.2	100
530 (B2U)--V	60.022	0	2.5	1.2	96.4	100
531 (EG)--V	60.039	0	8.5	4.6	86.9	100
532 (EG)--V	60.039	0	8.5	4.6	86.9	100
533 (A1G)--V	60.826	0.1	1.1	17.8	81	100
534 (B2G)--V	60.98	5.4	6.8	1.9	85.9	100
535 (B1U)--V	61.828	0	18	1.7	80.3	100
536 (EU)--V	62.234	0.1	1.8	26.5	71.6	100
537 (EU)--V	62.234	0.1	1.8	26.5	71.6	100
538 (EG)--V	62.867	0.6	15.3	8.6	75.5	100
539 (EG)--V	62.867	0.6	15.3	8.6	75.5	100
540 (A2G)--V	62.942	0	0.1	0	99.9	100
541 (EU)--V	63.313	0	0.2	0.3	99.4	100
542 (EU)--V	63.313	0	0.2	0.3	99.4	100
543 (B2G)--V	63.464	0	2.6	25.8	71.5	100
544 (B1G)--V	63.661	0	1.9	0.1	98.1	100
545 (B2G)--V	64.067	0.3	2.7	1.9	95	100
546 A1G)--V	65.069	2.4	17	2.3	78.2	100
547 (A1U)--V	65.069	0	2.6	6.7	90.7	100
548 (A2U)--V	65.209	0.2	8.7	19.1	72	100
549 (EU)--V	65.441	0.2	8.8	10.7	80.3	100
550 (EU)--V	65.441	0.2	8.8	10.7	80.3	100
551 (EG)--V	66.283	0	7.5	10	82.5	100
552 (EG)--V	66.283	0	7.5	10	82.5	100

553 (A1U)--V	67.35	0	13.6	12.4	73.9	100
554 (B1U)--V	67.487	0	12.2	8.3	79.5	100
555 (B1G)--V	68.341	0.8	57.9	4.6	36.7	100
556 A1G)--V	68.544	2.9	17.8	36.2	43	100
557 (A2G)--V	68.957	0	0.8	0.3	98.9	100
558 (EG)--V	69.263	0.3	7.3	10.9	81.5	100
559 (EG)--V	69.263	0.3	7.3	10.9	81.5	100
560 (EU)--V	69.369	0	0.6	0.8	98.6	100
561 (EU)--V	69.369	0	0.6	0.8	98.6	100
562 (B2G)--V	69.372	0	0.3	0.1	99.5	100
563 (EU)--V	69.547	0	13.9	8.7	77.4	100
564 (EU)--V	69.547	0	13.9	8.7	77.4	100
565 (B1G)--V	69.772	0	0.5	3.7	95.8	100
566 (EU)--V	69.961	0.1	26.3	25.6	47.9	100
567 (EU)--V	69.961	0.1	26.3	25.6	47.9	100
568 (A1G)--V	69.977	3	11.4	24	61.6	100
569 (B1U)--V	70.113	0	0.2	4.2	95.7	100
570 (A2G)--V	70.189	0	1.9	1.5	96.6	100
571 (EU)--V	70.288	0	10.7	8.5	80.7	100
572 (EU)--V	70.288	0	10.7	8.5	80.7	100
573 (B1G)--V	70.434	0	27	3.8	69.2	100
574 (A1G)--V	70.749	4.5	7.9	1.3	86.4	100
575 (B2U)--V	71.2	0	16	30.7	53.3	100
576 A1U)--V	71.364	0	5.4	16.6	78	100
577 (EG)--V	71.407	0.2	9.9	22	68	100
578 (EG)--V	71.407	0.2	9.9	22	68	100
579 (B1G)--V	71.426	0.2	24.4	3.7	71.7	100
580 (EU)--V	71.459	0.1	40.6	13.3	46	100
581 (EU)--V	71.459	0.1	40.6	13.3	46	100
582 (A1G)--V	71.643	0.1	54.5	19.6	25.8	100
583 (B2G)--V	72.513	0	0.3	8.6	91.1	100
584 (B2G)--V	72.752	0.1	4.1	21	74.8	100
585 (EU)--V	73.242	0	2	6.5	91.5	100
586 (EU)--V	73.242	0	2	6.5	91.5	100
587 (B1G)--V	73.52	1.2	53.2	5	40.7	100
588 (A2G)--V	73.592	0	0.9	6.6	92.6	100
589 (B2G)--V	74.102	0	0.1	0.4	99.5	100
590 (EU)--V	74.821	0	2.5	4.8	92.6	100
591 (EU)--V	74.821	0	2.5	4.8	92.6	100
592 (EU)--V	76.395	0.1	7.3	4.7	87.9	100
593 (EU)--V	76.395	0.1	7.3	4.7	87.9	100
594 (A2G)--V	76.549	0	1.2	2.6	96.2	100
595 (A1G)--V	76.822	0.2	21.3	25.1	53.4	100
596 (EU)--V	76.89	0.4	6.6	5.5	87.5	100
597 (EU)--V	76.89	0.4	6.6	5.5	87.5	100
598 (B1G)--V	78.385	0.8	6.2	5.8	87.2	100
599 (B2G)--V	78.443	0	0.1	7.5	92.3	100
600 (A2G)--V	79.464	0	0.4	0	99.6	100

601 A1G)--V	79.856	0.4	4	4.6	91	100
602 (EU)--V	79.999	0.1	9.5	10.7	79.8	100
603 (EU)--V	79.999	0.1	9.5	10.7	79.8	100
604 (A2G)--V	80.693	0	14.5	4.3	81.2	100
605 (B2G)--V	81.877	0	2.3	2.6	95.1	100
606 (EU)--V	82.342	0	1	4.9	94	100
607 (EU)--V	82.342	0	1	4.9	94	100
608 (EU)--V	84.751	0.2	7.3	19.6	73	100
609 (EU)--V	84.751	0.2	7.3	19.6	73	100
610 (B1G)--V	86	0.8	5.1	25.5	68.7	100
611 A1G)--V	87.937	0.4	4.2	54.9	40.5	100
612 (B2G)--V	88.48	0	1	1.8	97.2	100
613 (EU)--V	89.645	0	1.5	3	95.5	100
614 (EU)--V	89.645	0	1.5	3	95.5	100
615 (A2G)--V	90.297	0	8	13	79	100
616 A2G)--V	90.495	0	1	0.7	98.3	100
617 (EU)--V	92.347	0	5.3	4.2	90.5	100
618 (EU)--V	92.347	0	5.3	4.2	90.5	100
619 (B2G)--V	93.024	0	3.8	2.9	93.3	100

### VSXC Exchange Correlation Functional

Orbital	Index	E, eV	Zn	NZn	Nmeso	Pc	Total	
	1 A1G)--O	-9419.92		100	0	0	0	100
	2 (A1G)--O	-1139.04		100	0	0	0	100
	3 (A2U)--O	-1005.27		100	0	0	0	100
	4 (EU)--O	-1005.04		100	0	0	0	100
	5 (EU)--O	-1005.04		100	0	0	0	100
	6 (EU)--O	-384.049		0	99.8	0	0.2	100
	7 (EU)--O	-384.049		0	99.8	0	0.2	100
	8 (B1G)--O	-384.049		0	99.8	0	0.2	100
	9 (A1G)--O	-384.049		0	99.9	0	0.1	100
	10 (B2G)--O	-383.816		0	0	99.7	0.2	100
	11 (EU)--O	-383.816		0	0	99.8	0.2	100
	12 (EU)--O	-383.816		0	0	99.8	0.2	100
	13 (A1G)--O	-383.816		0	0	99.8	0.1	100
	14 (B2G)--O	-273.824		0	0	0.1	99.9	100
	15 (EU)--O	-273.823		0	0	0	99.9	100
	16 (EU)--O	-273.823		0	0	0	99.9	100
	17 (A1G)--O	-273.822		0	0	0	100	100
	18 (A2G)--O	-273.822		0	0	0	100	100
	19 (EU)--O	-273.822		0	0	0	100	100
	20 (EU)--O	-273.822		0	0	0	100	100
	21 B1G)--O	-273.822		0	0	0	100	100
	22 (EU)--O	-271.968		0	0	0	100	100
	23 (EU)--O	-271.968		0	0	0	100	100
	24 (A1G)--O	-271.968		0	0	0	100	100

25 (B1G)--O	-271.968	0	0	0	100	100
26 A2G)--O	-271.96	0	0	0	100	100
27 (EU)--O	-271.96	0	0	0	100	100
28 (EU)--O	-271.96	0	0	0	100	100
29 (B2G)--O	-271.96	0	0	0	100	100
30 (B1G)--O	-271.946	0	0	0	100	100
31 (EU)--O	-271.946	0	0	0	100	100
32 (EU)--O	-271.946	0	0	0	100	100
33 (A1G)--O	-271.946	0	0	0	100	100
34 (A2G)--O	-271.946	0	0	0	100	100
35 (EU)--O	-271.946	0	0	0	100	100
36 (EU)--O	-271.946	0	0	0	100	100
37 (B2G)--O	-271.946	0	0	0	100	100
38 (B1G)--O	-271.927	0	0	0	100	100
39 (EU)--O	-271.927	0	0	0	100	100
40 (EU)--O	-271.927	0	0	0	100	100
41 A1G)--O	-271.927	0	0	0	100	100
42 (A2G)--O	-271.919	0	0	0	100	100
43 (EU)--O	-271.919	0	0	0	100	100
44 (EU)--O	-271.919	0	0	0	100	100
45 (B2G)--O	-271.919	0	0	0	100	100
46 A1G)--O	-126.893	100	0	0	0	100
47 (A2U)--O	-84.097	100	0	0	0	100
48 (EU)--O	-83.73	100	0	0	0	100
49 (EU)--O	-83.73	100	0	0	0	100
50 (A1G)--O	-25.803	0.2	39	26.7	34.1	100
51 (EU)--O	-25.434	0.1	38.3	26.5	35.1	100
52 (EU)--O	-25.434	0.1	38.3	26.5	35.1	100
53 (B1G)--O	-24.679	0.1	60.4	0.8	38.7	100
54 (B2G)--O	-24.183	0	1.6	70.8	27.6	100
55 (EU)--O	-23.075	0	19.3	50.3	30.4	100
56 (EU)--O	-23.075	0	19.3	50.3	30.4	100
57 (A1G)--O	-22.239	0.1	18.2	50.2	31.5	100
58 (A1G)--O	-21.801	0.2	23.3	8.4	68.1	100
59 (EU)--O	-21.791	0	15.3	1.2	83.5	100
60 (EU)--O	-21.791	0	15.3	1.2	83.5	100
61 B1G)--O	-21.778	0.1	13.7	0	86.2	100
62 (A2G)--O	-19.706	0	2.7	6.2	91.1	100
63 (EU)--O	-19.365	0.1	13.6	4.1	82.2	100
64 (EU)--O	-19.365	0.1	13.6	4.1	82.2	100
65 (A1G)--O	-19.361	0.4	12.7	0.3	86.6	100
66 (EU)--O	-19.251	0	5.3	1.1	93.5	100
67 (EU)--O	-19.251	0	5.3	1.1	93.5	100
68 (B1G)--O	-19.248	0.3	19.7	0.6	79.4	100
69 (B2G)--O	-19.184	0	0	1.9	98.1	100
70 (A2G)--O	-18.303	0	6.3	9.5	84.2	100
71 (EU)--O	-17.588	0	8.1	19.6	72.3	100
72 (EU)--O	-17.588	0	8.1	19.6	72.3	100
73 (B1G)--O	-16.155	0.6	14.5	18.6	66.3	100
74 (A1G)--O	-15.99	1.1	11	0.4	87.5	100
75 (EU)--O	-15.863	0.2	10.8	0.3	88.7	100

76 (EU)--O	-15.863	0.2	10.8	0.3	88.7	100
77 (B2G)--O	-15.788	0	3.4	13.5	83.1	100
78 (B1G)--O	-15.564	0.3	3	12.4	84.3	100
79 (EU)--O	-14.972	0	5.6	3.9	90.5	100
80 (EU)--O	-14.972	0	5.6	3.9	90.5	100
81 B2G)--O	-14.811	1.3	31.1	22.3	45.4	100
82 (A2G)--O	-14.746	0	6.5	1.9	91.6	100
83 (A1G)--O	-13.8	2.2	8.6	1.6	87.6	100
84 (EU)--O	-13.716	0	20.6	15	64.4	100
85 (EU)--O	-13.716	0	20.6	15	64.4	100
86 (EU)--O	-13.25	0.2	15.1	18.8	65.8	100
87 (EU)--O	-13.25	0.2	15.1	18.8	65.8	100
88 (B1G)--O	-13.174	4.9	12.2	6	76.8	100
89 (A2G)--O	-12.479	0	29.5	17.3	53.2	100
90 (B2G)--O	-12.439	1	2.9	2.2	93.9	100
91 (EU)--O	-11.951	0	2.9	4	93	100
92 (EU)--O	-11.951	0	2.9	4	93	100
93 (A1G)--O	-11.887	14.4	20.1	1.3	64.2	100
94 (B1G)--O	-11.737	26.3	18.5	0.2	55	100
95 (A2U)--O	-11.497	0.6	26	18	55.4	100
96 (EU)--O	-11.491	0.4	13.1	1	85.5	100
97 (EU)--O	-11.491	0.4	13.1	1	85.5	100
98 (A2G)--O	-11.459	0	0.6	8	91.4	100
99 (EG)--O	-11.202	22.9	24.4	11.5	41.2	100
100 (EG)--O	-11.202	22.9	24.4	11.5	41.2	100
101 A1G)--O	-10.964	8.9	7.2	4.4	79.5	100
102 (B1G)--O	-10.867	27.8	11.1	1.7	59.4	100
103 (EU)--O	-10.816	0	1.2	1.7	97.1	100
104 (EU)--O	-10.816	0	1.2	1.7	97.1	100
105 (B2G)--O	-10.807	0.3	0.1	0.9	98.6	100
106 A1G)--O	-10.583	58	5.7	1.6	34.8	100
107 (A2G)--O	-10.537	0	0.6	3.9	95.5	100
108 (EU)--O	-10.456	0.2	5.6	4.5	89.7	100
109 (EU)--O	-10.456	0.2	5.6	4.5	89.7	100
110 (B2U)--O	-10.333	0	26.6	0	73.3	100
111 (EG)--O	-10.249	87.6	0.8	2.3	9.4	100
112 (EG)--O	-10.249	87.6	0.8	2.3	9.4	100
113 (B2G)--O	-10.119	56	5.1	0.9	38	100
114 (B1G)--O	-10.021	22.5	1.6	3.2	72.7	100
115 (A1G)--O	-9.524	49.4	17.6	3.6	29.4	100
116 B1U)--O	-9.437	0	0.1	51.1	48.9	100
117 (B2G)--O	-9.015	1.1	0.2	1.8	96.9	100
118 (EU)--O	-8.94	0	1.8	2.1	96.1	100
119 (EU)--O	-8.94	0	1.8	2.1	96.1	100
120 (EG)--O	-8.926	1.9	2.4	14.6	81.1	100
121 (EG)--O	-8.926	1.9	2.4	14.6	81.1	100
122 (A2U)--O	-8.912	0.4	7.4	3.8	88.4	100
123 (A2G)--O	-8.753	0	2.3	1.1	96.6	100
124 (A1G)--O	-8.565	0	1.1	2.3	96.6	100
125 (EU)--O	-8.56	2.6	31.2	2.1	64.2	100
126 (EU)--O	-8.56	2.6	31.2	2.1	64.2	100

127 (B2U)--O	-8.503	0	26.6	0	73.3	100
128 (B1G)--O	-8.229	2	0.6	3	94.4	100
129 (EU)--O	-8.177	2.3	23.5	7.2	67	100
130 (EU)--O	-8.177	2.3	23.5	7.2	67	100
131 (EG)--O	-7.798	2.7	20.4	21.2	55.8	100
132 (EG)--O	-7.798	2.7	20.4	21.2	55.8	100
133 (A1G)--O	-7.168	0.2	19.5	52.7	27.6	100
134 (A1U)--O	-6.761	0	0	0	99.9	100
135 (EU)--O	-6.463	0.1	18.7	49.3	31.9	100
136 (EU)--O	-6.463	0.1	18.7	49.3	31.9	100
137 (A2U)--O	-6.372	3.7	47.7	26.9	21.8	100
138 (B1U)--O	-6.254	0	0	5.3	94.7	100
139 (EG)--O	-6.232	0	0.5	10.2	89.3	100
140 (EG)--O	-6.232	0	0.5	10.2	89.3	100
141 A2U)--O	-6.139	0.1	2.6	34.2	63.1	100
142 (EG)--O	-6.034	1.8	28.9	1.7	67.6	100
143 (EG)--O	-6.034	1.8	28.9	1.7	67.6	100
144 (B2U)--O	-6.009	0	26.2	0	73.8	100
145 (B2G)--O	-5.982	0.6	11.8	60.3	27.2	100
146 B1G)--O	-5.63	25.5	51	0.7	22.7	100
147 (A1U)--O	-4.57	0	0.1	0.1	99.8	100
148 (EG)--V	-3.085	0.4	12.9	19.5	67.3	100
149 (EG)--V	-3.085	0.4	12.9	19.5	67.3	100
150 (B1U)--V	-1.605	0	0	25.2	74.8	100
151 B2U)--V	-1.382	0	19.3	0	80.6	100
152 (A2U)--V	-1.29	8.3	0.7	6	85	100
153 (EG)--V	-1.105	0.1	5.6	3.7	90.6	100
154 (EG)--V	-1.105	0.1	5.6	3.7	90.6	100
155 (A1U)--V	0.149	0	0	0	99.9	100
156 (EG)--V	0.205	0	1.7	0.9	97.3	100
157 (EG)--V	0.205	0	1.7	0.9	97.3	100
158 (A2U)--V	0.283	57.5	8.6	2.3	31.6	100
159 (A1G)--V	0.488	72.6	20.1	0	7.4	100
160 (B2U)--V	0.785	0	19.3	0.1	80.6	100
161 B1U)--V	0.982	0	0.1	18.5	81.5	100
162 (A1G)--V	2.09	0.3	0.1	2.4	97.2	100
163 (EU)--V	2.154	5.5	1.4	2.2	90.9	100
164 (EU)--V	2.154	5.5	1.4	2.2	90.9	100
165 (B1G)--V	2.305	0	0	0.1	99.9	100
166 (EG)--V	2.335	0.1	14.4	15.9	69.6	100
167 (EG)--V	2.335	0.1	14.4	15.9	69.6	100
168 (EU)--V	2.569	58.3	11.7	4.6	25.3	100
169 (EU)--V	2.569	58.3	11.7	4.6	25.3	100
170 (B2G)--V	3.079	0	0.9	0.5	98.6	100
171 A2U)--V	3.127	23.8	18.2	17	41	100
172 (EU)--V	3.307	0.3	1	0.5	98.3	100
173 (EU)--V	3.307	0.3	1	0.5	98.3	100
174 (A1G)--V	3.535	12.1	0.2	10.5	77.2	100
175 (A2G)--V	3.598	0	0.6	0.1	99.3	100
176 B2G)--V	3.974	0	0.1	6.2	93.7	100
177 (EU)--V	3.995	1.4	0.2	3	95.4	100



178 (EU)--V	3.995	1.4	0.2	3	95.4	100
179 (A1U)--V	4.087	0	0	0	100	100
180 (EG)--V	4.265	0	0.9	4.1	95.1	100
181 (EG)--V	4.265	0	0.9	4.1	95.1	100
182 (B1U)--V	4.278	0	0	4.6	95.4	100
183 (B1G)--V	4.366	0	4.1	0.1	95.7	100
184 (EU)--V	4.369	0.9	1.2	0.1	97.8	100
185 (EU)--V	4.369	0.9	1.2	0.1	97.8	100
186 A2G)--V	4.491	0	0.2	0	99.8	100
187 (A1G)--V	4.549	47	1.7	2.6	48.7	100
188 (B2G)--V	5.246	0.1	2.3	15.1	82.5	100
189 (EU)--V	5.33	7.3	8.9	5.1	78.7	100
190 (EU)--V	5.33	7.3	8.9	5.1	78.7	100
191 A1G)--V	5.498	0.1	0.6	1.5	97.9	100
192 (B1G)--V	5.536	0	30.2	3.7	66.1	100
193 (EU)--V	6.021	0.2	0.9	1.3	97.7	100
194 (EU)--V	6.021	0.2	0.9	1.3	97.7	100
195 (A2G)--V	6.171	0	6.6	0.5	93	100
196 A2U)--V	6.178	89.7	2.3	0.9	7.1	100
197 (B2G)--V	6.416	0	0.4	11.8	87.8	100
198 (EU)--V	6.477	0.7	0.3	5.7	93.3	100
199 (EU)--V	6.477	0.7	0.3	5.7	93.3	100
200 (A2G)--V	6.751	0	0.2	0	99.8	100
201 B1G)--V	6.758	0	2.1	0	97.9	100
202 (A1G)--V	7.135	8.8	8.9	18	64.3	100
203 (EU)--V	7.212	1.6	5.6	2.4	90.4	100
204 (EU)--V	7.212	1.6	5.6	2.4	90.4	100
205 (EU)--V	7.488	0.9	6.7	2.9	89.5	100
206 (EU)--V	7.488	0.9	6.7	2.9	89.5	100
207 (A1G)--V	7.681	7.6	0.7	5.1	86.6	100
208 (B1G)--V	8.227	0	0.4	0.1	99.6	100
209 (B2G)--V	8.239	0	0.5	2.1	97.4	100
210 (EU)--V	8.516	0.4	2.3	13	84.3	100
211 (EU)--V	8.516	0.4	2.3	13	84.3	100
212 (A1G)--V	8.772	0.4	2	2	95.6	100
213 (EU)--V	8.867	1.5	4.5	2.1	91.9	100
214 (EU)--V	8.867	1.5	4.5	2.1	91.9	100
215 (B2G)--V	8.929	0	4	25.3	70.6	100
216 B1G)--V	9.369	0	3.5	0.1	96.4	100
217 (B2G)--V	9.535	0	1.8	10.3	87.8	100
218 (A2G)--V	10.005	0	7.1	7.5	85.4	100
219 (EU)--V	10.023	2.7	3.5	18.3	75.5	100
220 (EU)--V	10.023	2.7	3.5	18.3	75.5	100
221 A1G)--V	10.146	1	16.8	13.4	68.8	100
222 (A2G)--V	10.918	0	0	1.1	98.9	100
223 (EU)--V	11.001	2.9	10.1	6.6	80.4	100
224 (EU)--V	11.001	2.9	10.1	6.6	80.4	100
225 (EU)--V	11.122	1.2	2.3	4.2	92.3	100
226 (EU)--V	11.122	1.2	2.3	4.2	92.3	100
227 (B1G)--V	11.313	0	20.6	7.8	71.6	100
228 (EU)--V	12.891	1.6	4	3.5	90.9	100

229 (EU)--V	12.891	1.6	4	3.5	90.9	100
230 (A2G)--V	13.029	0	0.2	5.9	93.8	100
231 B2G)--V	13.185	0	0.3	0.1	99.6	100
232 (EG)--V	13.489	0	1.7	1.4	96.8	100
233 (EG)--V	13.489	0	1.7	1.4	96.8	100
234 (B2U)--V	13.726	0	0.4	0	99.6	100
235 (A2U)--V	13.842	4	0.1	0.8	95.1	100
236 (EU)--V	14.034	0.4	0.4	2.4	96.8	100
237 (EU)--V	14.034	0.4	0.4	2.4	96.8	100
238 (A1G)--V	14.091	0.7	2.7	0.8	95.9	100
239 (EG)--V	14.405	0	2.7	1.6	95.7	100
240 (EG)--V	14.405	0	2.7	1.6	95.7	100
241 B1G)--V	14.438	0	34.3	5.2	60.4	100
242 (A2G)--V	14.47	0	0.6	1.6	97.9	100
243 (EU)--V	14.568	0.3	0.6	0.4	98.7	100
244 (EU)--V	14.568	0.3	0.6	0.4	98.7	100
245 (B2G)--V	14.651	0	0.4	1.7	97.9	100
246 B1U)--V	14.751	0	0	4.6	95.4	100
247 (B1G)--V	14.758	0	9.8	3.9	86.3	100
248 (EU)--V	14.919	0	0.6	1.4	97.9	100
249 (EU)--V	14.919	0	0.6	1.4	97.9	100
250 (B2G)--V	15.043	0	0.9	1.8	97.4	100
251 A1G)--V	15.158	2.1	0.7	14.1	83.2	100
252 (A2G)--V	15.224	0	0.4	1.3	98.3	100
253 (B2U)--V	15.371	0	1.3	0.1	98.6	100
254 (EU)--V	15.375	0.2	0.8	1.2	97.8	100
255 (EU)--V	15.375	0.2	0.8	1.2	97.8	100
256 A2U)--V	15.466	10.9	1.4	1.4	86.3	100
257 (B1G)--V	15.499	0	26.2	1.1	72.7	100
258 (EG)--V	15.72	0	0.5	2	97.4	100
259 (EG)--V	15.72	0	0.5	2	97.4	100
260 (A1U)--V	15.9	0	0	0	100	100
261 A1G)--V	16.001	1.2	0.4	17.7	80.7	100
262 (EU)--V	16.03	0.2	13.8	15	71	100
263 (EU)--V	16.03	0.2	13.8	15	71	100
264 (B1G)--V	16.176	0	0.4	0.7	99	100
265 (A2G)--V	16.188	0	1	1.5	97.5	100
266 (EU)--V	16.205	0.3	3.6	1.4	94.7	100
267 (EU)--V	16.205	0.3	3.6	1.4	94.7	100
268 (A1G)--V	16.307	1.7	18.6	2.9	76.8	100
269 (B2G)--V	16.308	0	0.6	8.2	91.2	100
270 (A1G)--V	16.48	0.3	20	17.5	62.2	100
271 (EU)--V	16.651	1.5	22.5	12.2	63.9	100
272 (EU)--V	16.651	1.5	22.5	12.2	63.9	100
273 (B1U)--V	16.728	0	0	1	99	100
274 (A2G)--V	16.852	0	1	3	96	100
275 (EG)--V	16.916	0	4.9	0.5	94.5	100
276 (EG)--V	16.916	0	4.9	0.5	94.5	100
277 (EU)--V	17.168	2.2	3.8	2.5	91.4	100
278 (EU)--V	17.168	2.2	3.8	2.5	91.4	100
279 (EU)--V	17.276	0.4	1	14.4	84.3	100

280 (EU)--V	17.276	0.4	1	14.4	84.3	100
281 B2G)--V	17.46	0	0.8	13.9	85.3	100
282 (EG)--V	17.649	0	1.4	4.2	94.4	100
283 (EG)--V	17.649	0	1.4	4.2	94.4	100
284 (A2U)--V	17.672	2.9	1.3	1.5	94.3	100
285 (B1G)--V	17.772	0.1	12.1	9	78.9	100
286 B2U)--V	17.793	0	2.1	0	97.9	100
287 (A1U)--V	17.923	0	0	0	100	100
288 (A1G)--V	18.447	6	24.3	3.5	66.2	100
289 (B1U)--V	18.563	0	0	2.8	97.2	100
290 (EG)--V	18.689	0	0.7	0.2	99.1	100
291 (EG)--V	18.689	0	0.7	0.2	99.1	100
292 (A2U)--V	18.842	0.7	0.3	4.7	94.3	100
293 (EU)--V	20.083	5.7	16	6.8	71.5	100
294 (EU)--V	20.083	5.7	16	6.8	71.5	100
295 (B2U)--V	20.223	0	1.2	0	98.8	100
296 (EG)--V	20.285	0	2.8	2.5	94.7	100
297 (EG)--V	20.285	0	2.8	2.5	94.7	100
298 (A1U)--V	20.563	0	0	0	100	100
299 (B1U)--V	21.013	0	0	3.9	96	100
300 (B2G)--V	21.1	0	0.2	3.7	96.2	100
301 (EG)--V	21.296	0.3	36.2	5.2	58.3	100
302 (EG)--V	21.296	0.3	36.2	5.2	58.3	100
303 (EU)--V	21.356	0.2	1.3	1.9	96.6	100
304 (EU)--V	21.356	0.2	1.3	1.9	96.6	100
305 (A1G)--V	21.39	0.1	0.4	1	98.5	100
306 B2G)--V	21.883	0	1.5	0.9	97.6	100
307 (A2G)--V	22.036	0	0.1	1.5	98.5	100
308 (EU)--V	22.072	0.1	0.1	1.1	98.7	100
309 (EU)--V	22.072	0.1	0.1	1.1	98.7	100
310 (A2U)--V	22.111	1.2	12.3	54.2	32.3	100
311 B1G)--V	22.441	0	0.4	0.2	99.4	100
312 (A2G)--V	22.449	0	1.3	0.5	98.2	100
313 (EU)--V	22.455	0	0.7	0.3	99	100
314 (EU)--V	22.455	0	0.7	0.3	99	100
315 (EG)--V	22.687	0	1.5	0.3	98.2	100
316 (EG)--V	22.687	0	1.5	0.3	98.2	100
317 (B2G)--V	23.01	0	11.6	11	77.4	100
318 (A1G)--V	23.107	0.5	8.3	6.8	84.4	100
319 (B2G)--V	23.202	0	2.5	4.4	93.1	100
320 (EU)--V	23.335	0.2	1.8	3.8	94.2	100
321 (EU)--V	23.335	0.2	1.8	3.8	94.2	100
322 (B1G)--V	23.745	0	0.3	0	99.7	100
323 (EU)--V	23.761	0.1	0.4	3.5	95.9	100
324 (EU)--V	23.761	0.1	0.4	3.5	95.9	100
325 (B2U)--V	23.798	0	67	0	32.9	100
326 A2G)--V	23.866	0	0.9	10.2	88.9	100
327 (A1G)--V	23.999	2.7	2.8	28.6	66	100
328 (A1U)--V	24.399	0	0	0	100	100
329 (B1G)--V	24.649	0	19.1	10.2	70.8	100
330 (EG)--V	24.711	0.1	13.3	42.5	44.1	100

331 (EG)--V	24.711	0.1	13.3	42.5	44.1	100
332 (A1G)--V	24.842	1	11	6.9	81.1	100
333 (B1U)--V	24.911	0	0	61.7	38.2	100
334 (EU)--V	25.023	0.4	3.7	7.6	88.3	100
335 (EU)--V	25.023	0.4	3.7	7.6	88.3	100
336 (EU)--V	25.423	0.4	9.4	5.1	85.1	100
337 (EU)--V	25.423	0.4	9.4	5.1	85.1	100
338 (A2G)--V	25.585	0	0	0	99.9	100
339 (B1G)--V	25.694	0	0.5	0.4	99.1	100
340 (EU)--V	26.043	0.4	0.2	3.6	95.9	100
341 (EU)--V	26.043	0.4	0.2	3.6	95.9	100
342 (A2U)--V	26.678	4.5	42.9	15.9	36.8	100
343 (B2G)--V	26.751	0	0.1	0.7	99.2	100
344 (A2G)--V	26.942	0	0	1.7	98.3	100
345 (EU)--V	26.965	0.1	1	2.4	96.5	100
346 (EU)--V	26.965	0.1	1	2.4	96.5	100
347 (B2G)--V	27.256	0	1.2	1.9	97	100
348 (B1G)--V	27.424	0	7.9	1.3	90.7	100
349 (EU)--V	27.547	0.4	5.8	3.1	90.6	100
350 (EU)--V	27.547	0.4	5.8	3.1	90.6	100
351 (A1G)--V	27.984	0	2.4	3.1	94.4	100
352 (EU)--V	28.077	0	6	5.7	88.3	100
353 (EU)--V	28.077	0	6	5.7	88.3	100
354 (A1G)--V	28.176	0.2	5.9	6.1	87.8	100
355 (B2G)--V	28.889	0	7.5	3.6	89	100
356 (EU)--V	29.247	0	1.9	2.3	95.8	100
357 (EU)--V	29.247	0	1.9	2.3	95.8	100
358 (A2G)--V	29.25	0	0.8	0.1	99.1	100
359 (A2G)--V	30.172	0	1.7	0.8	97.5	100
360 (B1G)--V	30.365	0	0.4	12.3	87.3	100
361 (EU)--V	30.386	0.1	0.7	1	98.1	100
362 (EU)--V	30.386	0.1	0.7	1	98.1	100
363 (B2G)--V	30.472	0	0.3	5.4	94.3	100
364 (B1G)--V	30.957	0	4.9	14.2	80.9	100
365 (EU)--V	31.25	0.2	5.7	3	91.2	100
366 (EU)--V	31.25	0.2	5.7	3	91.2	100
367 (A1G)--V	31.258	0.8	6.3	3.7	89.1	100
368 (B2G)--V	31.552	0	0.7	4.1	95.2	100
369 (B2U)--V	31.642	0	7.6	8	84.4	100
370 (EG)--V	32.06	0.1	4.8	15	80.1	100
371 (EG)--V	32.06	0.1	4.8	15	80.1	100
372 (A1G)--V	32.216	6.6	5	0.6	87.8	100
373 (EU)--V	32.498	0.9	6	4.9	88.2	100
374 (EU)--V	32.498	0.9	6	4.9	88.2	100
375 (A2G)--V	32.562	0	2.3	13.6	84.1	100
376 (A2U)--V	32.646	0.2	0.8	11.5	87.4	100
377 (B1G)--V	33.23	0.2	9	7.8	83	100
378 (EG)--V	33.622	0	8.8	10.2	81	100
379 (EG)--V	33.622	0	8.8	10.2	81	100
380 (A1U)--V	33.635	0	18.6	18	63.4	100
381 (B2U)--V	33.68	0	6.8	10	83.1	100

382 (EU)--V	33.746	0.2	4.1	6.8	88.9	100
383 (EU)--V	33.746	0.2	4.1	6.8	88.9	100
384 (B2G)--V	33.849	0	1.7	1.8	96.5	100
385 (B1U)--V	34.618	0	4.9	6.6	88.5	100
386 (EG)--V	34.687	0.2	4.9	6.8	88.1	100
387 (EG)--V	34.687	0.2	4.9	6.8	88.1	100
388 (EU)--V	34.792	0.2	2.1	13.9	83.8	100
389 (EU)--V	34.792	0.2	2.1	13.9	83.8	100
390 (A1U)--V	34.896	0	3.9	5.1	91	100
391 A2G)--V	35.37	0	0.6	8.2	91.2	100
392 (B1G)--V	35.383	0	0.5	5	94.5	100
393 (A2U)--V	35.644	4.3	28.1	17.5	50.1	100
394 (EG)--V	35.663	1.9	18.8	7.9	71.3	100
395 (EG)--V	35.663	1.9	18.8	7.9	71.3	100
396 A1G)--V	36.291	3.3	5.3	0.1	91.3	100
397 (EU)--V	36.409	0.1	4	0.5	95.4	100
398 (EU)--V	36.409	0.1	4	0.5	95.4	100
399 (B1G)--V	36.743	0	6.5	0.2	93.3	100
400 (EU)--V	37.288	0.3	7.2	0.2	92.3	100
401 (EU)--V	37.288	0.3	7.2	0.2	92.3	100
402 (B2U)--V	37.319	0	28.3	0.6	71.1	100
403 (EG)--V	37.983	0.1	2.1	4.3	93.5	100
404 (EG)--V	37.983	0.1	2.1	4.3	93.5	100
405 (A2U)--V	37.989	0.4	1.4	2.1	96	100
406 A1G)--V	38.012	0	0.3	0	99.6	100
407 (B2U)--V	38.046	0	0.3	0.6	99.1	100
408 (EU)--V	38.367	0.1	1.9	1.6	96.4	100
409 (EU)--V	38.367	0.1	1.9	1.6	96.4	100
410 (EG)--V	38.39	0.4	11.7	12.2	75.7	100
411 (EG)--V	38.39	0.4	11.7	12.2	75.7	100
412 (B1G)--V	38.41	0	0.1	1.1	98.7	100
413 (A2U)--V	38.584	2.3	10.4	0.5	86.8	100
414 (A2G)--V	38.666	0	3.4	16.5	80	100
415 (B2G)--V	38.727	0	0.1	0.4	99.5	100
416 B2U)--V	38.912	0	2.2	0.7	97	100
417 (B1U)--V	39.014	0	15.1	20.1	64.8	100
418 (EG)--V	39.187	0.1	2.9	1.5	95.5	100
419 (EG)--V	39.187	0.1	2.9	1.5	95.5	100
420 (A1U)--V	39.21	0	0	0	100	100
421 B1U)--V	39.3	0	7.6	10.8	81.5	100
422 (EG)--V	39.354	0.7	18.7	12	68.7	100
423 (EG)--V	39.354	0.7	18.7	12	68.7	100
424 (A2U)--V	40.247	8.2	39.8	6	46	100
425 (EU)--V	40.451	0	1.3	0.7	98	100
426 (EU)--V	40.451	0	1.3	0.7	98	100
427 (A2G)--V	41.039	0	4.2	0.1	95.7	100
428 (A2G)--V	42.147	0	2.6	3.4	94	100
429 (EU)--V	42.539	0.5	8	0.3	91.1	100
430 (EU)--V	42.539	0.5	8	0.3	91.1	100
431 A1G)--V	42.676	0.2	37.1	0.7	62.1	100
432 (B2G)--V	42.8	0	0	3.8	96.1	100

433 (EU)--V	43.097	0.3	5.5	1.6	92.7	100
434 (EU)--V	43.097	0.3	5.5	1.6	92.7	100
435 (A1G)--V	43.883	0.3	43.7	1.2	54.8	100
436 B1G)--V	44.113	0	29.6	1.9	68.5	100
437 (B2G)--V	45.244	0	0.2	12.7	87.1	100
438 (EU)--V	45.783	1.1	4.2	37.3	57.5	100
439 (EU)--V	45.783	1.1	4.2	37.3	57.5	100
440 (A1G)--V	46.236	1.1	0.8	50.6	47.6	100
441 B1G)--V	46.502	0	44.1	9.9	46	100
442 (EU)--V	46.789	0.1	38.4	5.1	56.3	100
443 (EU)--V	46.789	0.1	38.4	5.1	56.3	100
444 (A1G)--V	46.961	0.6	46.4	4.2	48.8	100
445 (B1U)--V	46.985	0	1.4	12.1	86.5	100
446 (EG)--V	47.342	0	2.4	9.6	88	100
447 (EG)--V	47.342	0	2.4	9.6	88	100
448 (A1U)--V	47.841	0	3.3	2.4	94.2	100
449 (B1G)--V	48.187	0	51.7	0.1	48.1	100
450 (EU)--V	48.549	0.3	17.4	1.1	81.1	100
451 (EU)--V	48.549	0.3	17.4	1.1	81.1	100
452 (B2G)--V	48.712	0	0.2	22.4	77.4	100
453 (A1G)--V	48.863	0.3	16.4	15.3	68.1	100
454 (A2G)--V	49.024	0	0.4	0	99.6	100
455 (EU)--V	49.067	0.1	0.3	32.9	66.6	100
456 (EU)--V	49.067	0.1	0.3	32.9	66.6	100
457 (A2U)--V	49.241	0.5	10.7	24.6	64.1	100
458 (A1G)--V	49.448	0.7	24.4	24.6	50.2	100
459 (EU)--V	50.012	0	18.3	5.9	75.8	100
460 (EU)--V	50.012	0	18.3	5.9	75.8	100
461 B1G)--V	50.099	0	36.3	4.8	58.9	100
462 (EG)--V	50.303	0.3	15.5	17.2	67	100
463 (EG)--V	50.303	0.3	15.5	17.2	67	100
464 (A1G)--V	50.543	0.3	14.2	42.9	42.6	100
465 (A2G)--V	50.648	0	0	0.1	99.9	100
466 (EU)--V	50.914	0	1.1	2.3	96.5	100
467 (EU)--V	50.914	0	1.1	2.3	96.5	100
468 (B1G)--V	51.057	0	17.9	3.5	78.6	100
469 (B2G)--V	51.113	0	0	0.3	99.7	100
470 (EU)--V	51.281	0.1	0.2	1.3	98.4	100
471 (EU)--V	51.281	0.1	0.2	1.3	98.4	100
472 (B2U)--V	51.338	0	24.8	10.5	64.7	100
473 (EU)--V	51.741	6.1	15.5	15.7	62.7	100
474 (EU)--V	51.741	6.1	15.5	15.7	62.7	100
475 (B1G)--V	51.838	0	18.9	5.9	75.1	100
476 (EU)--V	52.424	7.6	29.6	3.2	59.6	100
477 (EU)--V	52.424	7.6	29.6	3.2	59.6	100
478 (A1G)--V	53.012	0.5	7.1	14.5	77.9	100
479 (B2G)--V	53.167	0	0.3	10.4	89.3	100
480 (A2G)--V	53.207	0	0.1	0.6	99.3	100
481 B2U)--V	53.659	0	28.7	14.9	56.4	100
482 (EU)--V	53.89	0	6.2	1.9	91.9	100
483 (EU)--V	53.89	0	6.2	1.9	91.9	100

484 (A1G)--V	54.515	0	19.3	17.4	63.3	100
485 (EU)--V	54.702	0.2	4.5	2.4	92.9	100
486 (EU)--V	54.702	0.2	4.5	2.4	92.9	100
487 (EG)--V	54.888	0.9	28.3	17.8	53	100
488 (EG)--V	54.888	0.9	28.3	17.8	53	100
489 (B1G)--V	55.068	0	27.9	3.4	68.7	100
490 (B1U)--V	56.032	0	2.4	28.9	68.7	100
491 A2U)--V	56.065	0.4	5	20.8	73.9	100
492 (EG)--V	56.081	3.3	5.1	20	71.6	100
493 (EG)--V	56.081	3.3	5.1	20	71.6	100
494 (A2G)--V	56.09	0	11.4	5.1	83.5	100
495 (A1U)--V	56.108	0	24.2	10.9	64.8	100
496 B2G)--V	56.247	0	0.2	0.2	99.7	100
497 (EU)--V	56.51	0.1	1	1.5	97.4	100
498 (EU)--V	56.51	0.1	1	1.5	97.4	100
499 (EU)--V	57.093	0	2.3	4.3	93.3	100
500 (EU)--V	57.093	0	2.3	4.3	93.3	100
501 A2G)--V	57.175	0	3.1	2.7	94.2	100
502 (B1G)--V	57.564	0	6.5	10.2	83.4	100
503 (B2G)--V	57.753	0	0.3	5.8	93.9	100
504 (EU)--V	57.962	0	0.6	3.4	96	100
505 (EU)--V	57.962	0	0.6	3.4	96	100
506 A1G)--V	58.219	0.6	4	0.7	94.6	100
507 (EG)--V	58.224	34.5	14.1	1.2	50.2	100
508 (EG)--V	58.224	34.5	14.1	1.2	50.2	100
509 (B1U)--V	58.691	0	8.7	13.9	77.4	100
510 (EG)--V	58.841	44	8.7	4.1	43.1	100
511 (EG)--V	58.841	44	8.7	4.1	43.1	100
512 (A1U)--V	59.512	0	5.8	5	89.2	100
513 (B2U)--V	59.67	0	1.1	0	98.9	100
514 (A2G)--V	60.001	0	0.1	0.2	99.7	100
515 (EU)--V	60.169	0.1	4	6.3	89.6	100
516 (EU)--V	60.169	0.1	4	6.3	89.6	100
517 (EG)--V	60.266	0.1	9.8	0.1	90.1	100
518 (EG)--V	60.266	0.1	9.8	0.1	90.1	100
519 (B1U)--V	60.355	0	7.2	1.3	91.5	100
520 (EG)--V	60.57	2.1	1.4	6.9	89.6	100
521 (EG)--V	60.57	2.1	1.4	6.9	89.6	100
522 (A2U)--V	60.683	0.3	32.2	6.2	61.3	100
523 (A2U)--V	60.784	0.1	11.3	1	87.6	100
524 (A2G)--V	60.892	0	1.9	0.8	97.4	100
525 (A1U)--V	60.919	0	0.2	4.9	94.9	100
526 B2G)--V	61.092	0	0.2	11.5	88.3	100
527 (EU)--V	61.527	2.2	12.3	14.6	70.9	100
528 (EU)--V	61.527	2.2	12.3	14.6	70.9	100
529 (B2U)--V	61.822	0	2.4	1.1	96.4	100
530 (EG)--V	61.832	0	8.4	4.4	87.2	100
531 (EG)--V	61.832	0	8.4	4.4	87.2	100
532 (B1G)--V	61.925	0	36.7	16.2	47.1	100
533 (A1G)--V	62.688	0.1	1.1	16.4	82.5	100
534 (B2G)--V	63.12	4.8	4.9	4.4	85.8	100

535 (B1U)--V	63.702	0	18.1	1.9	80.1	100
536 (EU)--V	64.182	0.1	1.4	22.6	75.8	100
537 (EU)--V	64.182	0.1	1.4	22.6	75.8	100
538 (EG)--V	64.756	0.6	15.5	8.8	75.1	100
539 (EG)--V	64.756	0.6	15.5	8.8	75.1	100
540 (A2G)--V	64.999	0	0.1	0	99.9	100
541 B1G)--V	65.282	0	1	0.2	98.7	100
542 (EU)--V	65.337	0	0.3	1.5	98.2	100
543 (EU)--V	65.337	0	0.3	1.5	98.2	100
544 (B2G)--V	65.839	0	2.4	25.7	71.8	100
545 (B2G)--V	66.092	0.5	4.6	2.9	92.1	100
546 A1G)--V	66.84	1.9	16	0.9	81.3	100
547 (A1U)--V	66.972	0	2.7	6.8	90.4	100
548 (A2U)--V	67.113	0.1	8.6	19.4	71.8	100
549 (EU)--V	67.194	0.3	9.6	14.2	75.9	100
550 (EU)--V	67.194	0.3	9.6	14.2	75.9	100
551 (EG)--V	68.239	0	7.7	10.2	82	100
552 (EG)--V	68.239	0	7.7	10.2	82	100
553 (A1U)--V	69.365	0	13.5	12.3	74.2	100
554 (B1U)--V	69.49	0	12.5	8.5	79	100
555 (B1G)--V	70.621	0.7	51.1	5.9	42.3	100
556 A1G)--V	70.736	3.1	18.3	36.7	41.9	100
557 (B2G)--V	71.017	0	0.4	0.1	99.5	100
558 (A2G)--V	71.093	0	0.4	0.1	99.6	100
559 (EU)--V	71.122	0	0.1	0.2	99.6	100
560 (EU)--V	71.122	0	0.1	0.2	99.6	100
561 (EG)--V	71.29	0.3	7.2	10.9	81.6	100
562 (EG)--V	71.29	0.3	7.2	10.9	81.6	100
563 (EU)--V	71.738	0.2	25.5	20.1	54.2	100
564 (EU)--V	71.738	0.2	25.5	20.1	54.2	100
565 (A2G)--V	71.929	0	6.3	4.5	89.2	100
566 (EU)--V	72.081	0.1	7.9	13.8	78.3	100
567 (EU)--V	72.081	0.1	7.9	13.8	78.3	100
568 (B1G)--V	72.127	0	0.4	5.3	94.3	100
569 (B1U)--V	72.155	0	0.1	4.1	95.7	100
570 (A1G)--V	72.286	2.7	7.7	16.9	72.7	100
571 (EU)--V	72.567	0	7	5.2	87.7	100
572 (EU)--V	72.567	0	7	5.2	87.7	100
573 (B1G)--V	72.655	0	31	1.9	67.1	100
574 (A1G)--V	73.003	5.6	8.5	0.5	85.3	100
575 (B2U)--V	73.292	0	15.9	30.9	53.2	100
576 A1U)--V	73.46	0	5.6	16.8	77.6	100
577 (EG)--V	73.502	0.2	9.9	22.2	67.7	100
578 (EG)--V	73.502	0.2	9.9	22.2	67.7	100
579 (B1G)--V	73.848	0.3	27	3.9	68.8	100
580 (EU)--V	73.884	0.1	41.2	16.5	42.2	100
581 (EU)--V	73.884	0.1	41.2	16.5	42.2	100
582 (A1G)--V	74.005	0.2	50.1	23.4	26.4	100
583 (B2G)--V	74.77	0.1	0.9	13.1	86	100
584 (B2G)--V	74.979	0.1	4.4	14.2	81.3	100
585 (EU)--V	75.629	0	2.7	7.2	90.1	100



586 (EU)--V	75.629	0	2.7	7.2	90.1	100
587 (B1G)--V	75.781	1	52.9	4.2	41.9	100
588 (A2G)--V	75.958	0	1	6.4	92.6	100
589 (B2G)--V	76.392	0	0.1	0.3	99.6	100
590 (EU)--V	77.129	0	2.6	4.4	93	100
591 (EU)--V	77.129	0	2.6	4.4	93	100
592 (EU)--V	78.692	0.1	7.8	4.7	87.4	100
593 (EU)--V	78.692	0.1	7.8	4.7	87.4	100
594 (A2G)--V	79.047	0	1.2	2.6	96.3	100
595 (EU)--V	79.191	0.4	6.6	5.7	87.3	100
596 (EU)--V	79.191	0.4	6.6	5.7	87.3	100
597 (A1G)--V	79.196	0.2	20.7	25.5	53.6	100
598 (B1G)--V	80.625	0.9	7	6	86.2	100
599 (B2G)--V	80.984	0	0.1	8.1	91.7	100
600 (A2G)--V	82.065	0	0.3	0	99.7	100
601 A1G)--V	82.093	0.4	3.9	5	90.8	100
602 (EU)--V	82.589	0.1	9.1	10	80.8	100
603 (EU)--V	82.589	0.1	9.1	10	80.8	100
604 (A2G)--V	83.26	0	16.8	5	78.2	100
605 (B2G)--V	84.315	0	2.3	3.2	94.5	100
606 (EU)--V	84.787	0	0.9	4.9	94.1	100
607 (EU)--V	84.787	0	0.9	4.9	94.1	100
608 (EU)--V	87.269	0.2	7.4	19.4	73	100
609 (EU)--V	87.269	0.2	7.4	19.4	73	100
610 (B1G)--V	88.504	0.7	5.4	25.4	68.5	100
611 A1G)--V	90.498	0.4	3.5	55.7	40.5	100
612 (B2G)--V	90.903	0	0.8	1.6	97.6	100
613 (EU)--V	92.093	0	1.1	2.6	96.3	100
614 (EU)--V	92.093	0	1.1	2.6	96.3	100
615 (A2G)--V	92.771	0	0	0.4	99.6	100
616 A2G)--V	93.123	0	7.7	11.1	81.2	100
617 (EU)--V	95.011	0	6	5	88.9	100
618 (EU)--V	95.011	0	6	5	88.9	100
619 (B2G)--V	95.677	0	4.3	3.5	92.2	100

### BLYP Exchange Correlation Functional

Orbital	Index	E, eV	Zn	NZn	Nmeso	Pc	Total
	1 A1G)--O	-9409.74	100	0	0	0	100
	2 (A1G)--O	-1133.98	100	0	0	0	100
	3 (A2U)--O	-1000.32	100	0	0	0	100
	4 (EU)--O	-1000.12	100	0	0	0	100
	5 (EU)--O	-1000.12	100	0	0	0	100
	6 (EU)--O	-381.871	0	99.8	0	0.2	100
	7 (EU)--O	-381.871	0	99.8	0	0.2	100
	8 (B1G)--O	-381.871	0	99.7	0	0.2	100
	9 (A1G)--O	-381.871	0	99.9	0	0.1	100
	10 (B2G)--O	-381.617	0	0	99.7	0.3	100
	11 (EU)--O	-381.617	0	0	99.7	0.3	100

12 (EU)--O	-381.617	0	0	99.7	0.3	100
13 (A1G)--O	-381.617	0	0	99.8	0.2	100
14 (B2G)--O	-271.842	0	0	0.2	99.8	100
15 (EU)--O	-271.842	0	0	0.1	99.9	100
16 (EU)--O	-271.842	0	0	0.1	99.9	100
17 (A1G)--O	-271.841	0	0	0	100	100
18 (A2G)--O	-271.841	0	0	0	100	100
19 (EU)--O	-271.84	0	0	0	100	100
20 (EU)--O	-271.84	0	0	0	100	100
21 B1G)--O	-271.84	0	0	0	100	100
22 (B1G)--O	-270.073	0	0	0	100	100
23 (EU)--O	-270.073	0	0	0	100	100
24 (EU)--O	-270.073	0	0	0	100	100
25 (A1G)--O	-270.073	0	0	0	100	100
26 A2G)--O	-270.073	0	0	0	100	100
27 (EU)--O	-270.073	0	0	0	100	100
28 (EU)--O	-270.073	0	0	0	100	100
29 (B2G)--O	-270.073	0	0	0	100	100
30 (B1G)--O	-270.065	0	0	0	100	100
31 (EU)--O	-270.065	0	0	0	100	100
32 (EU)--O	-270.065	0	0	0	100	100
33 (A1G)--O	-270.065	0	0	0	100	100
34 (A2G)--O	-270.06	0	0	0	100	100
35 (EU)--O	-270.06	0	0	0	100	100
36 (EU)--O	-270.06	0	0	0	100	100
37 (B2G)--O	-270.06	0	0	0	100	100
38 (EU)--O	-270.05	0	0	0	100	100
39 (EU)--O	-270.05	0	0	0	100	100
40 (A1G)--O	-270.05	0	0	0	100	100
41 B1G)--O	-270.05	0	0	0	100	100
42 (A2G)--O	-270.044	0	0	0	100	100
43 (EU)--O	-270.044	0	0	0	100	100
44 (EU)--O	-270.044	0	0	0	100	100
45 (B2G)--O	-270.044	0	0	0	100	100
46 A1G)--O	-124.622	100	0	0	0	100
47 (A2U)--O	-82.269	100	0	0	0	100
48 (EU)--O	-81.953	100	0	0	0	100
49 (EU)--O	-81.953	100	0	0	0	100
50 (A1G)--O	-24.725	0.4	39.2	25.2	35.2	100
51 (EU)--O	-24.358	0.2	38.4	24.9	36.5	100
52 (EU)--O	-24.358	0.2	38.4	24.9	36.5	100
53 (B1G)--O	-23.645	0.1	58.5	0.8	40.6	100
54 (B2G)--O	-23.093	0	1.8	69.3	28.9	100
55 (EU)--O	-22.047	0	18	49.5	32.5	100
56 (EU)--O	-22.047	0	18	49.5	32.5	100
57 (A1G)--O	-21.25	0.1	17.3	49.7	32.8	100
58 (A1G)--O	-20.801	0.3	20.8	7.2	71.7	100
59 (EU)--O	-20.782	0.1	14	1.1	84.9	100
60 (EU)--O	-20.782	0.1	14	1.1	84.9	100
61 B1G)--O	-20.768	0.1	12.5	0	87.4	100
62 (A2G)--O	-18.753	0	2.8	6.5	90.7	100

63 (A1G)--O	-18.439	0.6	12.5	0.3	86.6	100
64 (EU)--O	-18.414	0.1	13.1	4.1	82.7	100
65 (EU)--O	-18.414	0.1	13.1	4.1	82.7	100
66 (EU)--O	-18.305	0.1	4.9	1.2	93.9	100
67 (EU)--O	-18.305	0.1	4.9	1.2	93.9	100
68 (B1G)--O	-18.292	0.4	18.7	0.6	80.3	100
69 (B2G)--O	-18.232	0	0	1.8	98.2	100
70 (A2G)--O	-17.41	0	5.5	8.3	86.2	100
71 (EU)--O	-16.753	0	6.8	18	75.2	100
72 (EU)--O	-16.753	0	6.8	18	75.2	100
73 (B1G)--O	-15.415	0.7	11.1	19.7	68.5	100
74 (A1G)--O	-15.306	2	11.6	0.5	85.8	100
75 (EU)--O	-15.145	0.2	11.2	0.4	88.1	100
76 (EU)--O	-15.145	0.2	11.2	0.4	88.1	100
77 (B2G)--O	-14.987	0	3	13.9	83.1	100
78 (B1G)--O	-14.899	0.5	5.8	10	83.7	100
79 (EU)--O	-14.278	0	5.8	3.2	91	100
80 (EU)--O	-14.278	0	5.8	3.2	91	100
81 B2G)--O	-14.186	1.5	30.7	23	44.7	100
82 (A2G)--O	-14.043	0	5.4	1.5	93.1	100
83 (A1G)--O	-13.29	3.2	8	1.4	87.4	100
84 (EU)--O	-13.135	0	17.8	13.3	68.9	100
85 (EU)--O	-13.135	0	17.8	13.3	68.9	100
86 (EU)--O	-12.734	0.4	13.2	18.2	68.2	100
87 (EU)--O	-12.734	0.4	13.2	18.2	68.2	100
88 (B1G)--O	-12.704	5.4	12.8	5.5	76.3	100
89 (A2G)--O	-11.948	0	22.6	13.7	63.7	100
90 (B2G)--O	-11.892	0.8	1.9	1.5	95.8	100
91 A1G)--O	-11.515	19.3	20.1	1.5	59.2	100
92 (EU)--O	-11.42	0	2.4	3.7	93.9	100
93 (EU)--O	-11.42	0	2.4	3.7	93.9	100
94 (B1G)--O	-11.327	31.4	18.8	0.2	49.6	100
95 (EU)--O	-10.993	0.6	13.8	1.2	84.4	100
96 (EU)--O	-10.993	0.6	13.8	1.2	84.4	100
97 (A2U)--O	-10.982	0.6	25.1	17.8	56.5	100
98 (A2G)--O	-10.937	0	0.5	6.6	92.9	100
99 (EG)--O	-10.703	21.2	24.4	11.6	42.8	100
100 (EG)--O	-10.703	21.2	24.4	11.6	42.8	100
101 A1G)--O	-10.482	7.1	8.1	6.1	78.7	100
102 (B1G)--O	-10.426	22.5	10.7	1.8	65	100
103 (B2G)--O	-10.383	0.3	0.1	0.7	98.9	100
104 (EU)--O	-10.378	0	1.1	1.3	97.6	100
105 (EU)--O	-10.378	0	1.1	1.3	97.6	100
106 A1G)--O	-10.119	44.5	5.5	2.1	48	100
107 (A2G)--O	-10.108	0	0.7	3.9	95.4	100
108 (EU)--O	-9.995	0.3	5	4.5	90.3	100
109 (EU)--O	-9.995	0.3	5	4.5	90.3	100
110 (B2U)--O	-9.865	0	26.4	0	73.6	100
111 (EG)--O	-9.713	87.2	1.1	2.2	9.5	100
112 (EG)--O	-9.713	87.2	1.1	2.2	9.5	100
113 (B2G)--O	-9.623	50.5	6.2	0.8	42.5	100

114 (B1G)--O	-9.608	16.8	1.2	3.1	78.9	100
115 (A1G)--O	-9.09	61.7	12.3	2.4	23.6	100
116 B1U)--O	-9.013	0	0	50.5	49.5	100
117 (B2G)--O	-8.625	1.4	0.2	1.5	96.8	100
118 (EU)--O	-8.553	0	1.4	1.7	97	100
119 (EU)--O	-8.553	0	1.4	1.7	97	100
120 (EG)--O	-8.495	2	2	14.9	81	100
121 (EG)--O	-8.495	2	2	14.9	81	100
122 (A2U)--O	-8.475	0.4	7.1	3.9	88.7	100
123 (A2G)--O	-8.362	0	1.9	1.1	97	100
124 (A1G)--O	-8.205	0	1.6	3	95.4	100
125 (EU)--O	-8.184	4	28.1	2.2	65.7	100
126 (EU)--O	-8.184	4	28.1	2.2	65.7	100
127 (B2U)--O	-8.094	0	25.7	0	74.3	100
128 (B1G)--O	-7.855	1.7	0.6	3	94.8	100
129 (EU)--O	-7.813	3.5	21.2	6.7	68.6	100
130 (EU)--O	-7.813	3.5	21.2	6.7	68.6	100
131 (EG)--O	-7.43	3.1	19.7	20.1	57.2	100
132 (EG)--O	-7.43	3.1	19.7	20.1	57.2	100
133 (A1G)--O	-6.674	0.2	19	53.6	27.2	100
134 (A1U)--O	-6.449	0	0	0	99.9	100
135 (A2U)--O	-6.022	3.4	47.5	24.2	25	100
136 (EU)--O	-6.012	0.2	17.4	49.2	33.2	100
137 (EU)--O	-6.012	0.2	17.4	49.2	33.2	100
138 (B1U)--O	-5.956	0	0	5.3	94.7	100
139 (EG)--O	-5.934	0	0.5	10.1	89.4	100
140 (EG)--O	-5.934	0	0.5	10.1	89.4	100
141 A2U)--O	-5.833	0.1	3.8	36.6	59.5	100
142 (EG)--O	-5.723	2	28.6	1.6	67.8	100
143 (EG)--O	-5.723	2	28.6	1.6	67.8	100
144 (B2U)--O	-5.71	0	25.9	0	74.1	100
145 (B2G)--O	-5.549	0.7	11.5	60	27.8	100
146 B1G)--O	-5.087	24.4	48.8	0.8	26	100
147 (A1U)--O	-4.382	0	0.1	0.1	99.8	100
148 (EG)--V	-2.934	0.4	13.3	19.8	66.5	100
149 (EG)--V	-2.934	0.4	13.3	19.8	66.5	100
150 (B1U)--V	-1.521	0	0	25.2	74.8	100
151 B2U)--V	-1.308	0	19.6	0	80.4	100
152 (A2U)--V	-1.192	7.5	0.8	5.7	86	100
153 (EG)--V	-1.038	0.1	5.6	3.7	90.6	100
154 (EG)--V	-1.038	0.1	5.6	3.7	90.6	100
155 (A1U)--V	0.131	0	0	0	100	100
156 (EG)--V	0.19	0	1.7	0.9	97.3	100
157 (EG)--V	0.19	0	1.7	0.9	97.3	100
158 (A2U)--V	0.275	62.3	8.7	1.8	27.3	100
159 (A1G)--V	0.49	73	16.4	0.3	10.4	100
160 (B2U)--V	0.743	0	19.4	0.1	80.5	100
161 B1U)--V	0.938	0	0.1	18.5	81.5	100
162 (A1G)--V	2.051	0.3	0.1	1.4	98.2	100
163 (EU)--V	2.083	17.5	2.3	1.2	78.9	100
164 (EU)--V	2.083	17.5	2.3	1.2	78.9	100

165 (EG)--V	2.211	0.1	14.4	16	69.5	100
166 (EG)--V	2.211	0.1	14.4	16	69.5	100
167 (B1G)--V	2.232	0	0	0.1	99.9	100
168 (EU)--V	2.312	51.9	5.3	1.2	41.7	100
169 (EU)--V	2.312	51.9	5.3	1.2	41.7	100
170 (A2U)--V	2.809	30.5	15.6	16.1	37.8	100
171 B2G)--V	3.019	0	0.8	0.1	99.1	100
172 (EU)--V	3.219	0.1	0.9	0.2	98.8	100
173 (EU)--V	3.219	0.1	0.9	0.2	98.8	100
174 (A1G)--V	3.357	29.6	0.4	9.4	60.6	100
175 (A2G)--V	3.464	0	0.6	0.1	99.3	100
176 A1U)--V	3.845	0	0	0	100	100
177 (EU)--V	3.906	0.9	0.1	2.6	96.5	100
178 (EU)--V	3.906	0.9	0.1	2.6	96.5	100
179 (B2G)--V	3.956	0	0	3.5	96.4	100
180 (EG)--V	4.021	0	0.9	4.1	95	100
181 (EG)--V	4.021	0	0.9	4.1	95	100
182 (B1U)--V	4.043	0	0	4.6	95.3	100
183 (A1G)--V	4.165	36.2	1.1	0.3	62.3	100
184 (B1G)--V	4.301	0	3.5	0.1	96.4	100
185 (EU)--V	4.31	0.5	1.2	0.1	98.1	100
186 (EU)--V	4.31	0.5	1.2	0.1	98.1	100
187 (A2G)--V	4.446	0	0.1	0	99.9	100
188 (EU)--V	5.121	6.2	11.2	4.9	77.7	100
189 (EU)--V	5.121	6.2	11.2	4.9	77.7	100
190 (B2G)--V	5.183	0.1	3.4	13.8	82.7	100
191 B1G)--V	5.357	0	30.5	3.7	65.8	100
192 (A1G)--V	5.441	0.1	0.5	1	98.4	100
193 (A2U)--V	5.657	87.5	3.3	1.2	8	100
194 (EU)--V	5.932	0.2	0.6	2.3	96.8	100
195 (EU)--V	5.932	0.2	0.6	2.3	96.8	100
196 A2G)--V	6.028	0	6.5	0.6	92.9	100
197 (B2G)--V	6.273	0	0.4	12.7	86.9	100
198 (EU)--V	6.279	0.9	0.3	6	92.7	100
199 (EU)--V	6.279	0.9	0.3	6	92.7	100
200 (A2G)--V	6.589	0	0.2	0	99.7	100
201 B1G)--V	6.604	0	2.4	0	97.6	100
202 (A1G)--V	6.839	9.1	10.4	22.7	57.8	100
203 (EU)--V	6.932	1.5	6.2	2.7	89.5	100
204 (EU)--V	6.932	1.5	6.2	2.7	89.5	100
205 (EU)--V	7.274	0.9	6.1	2.5	90.5	100
206 (EU)--V	7.274	0.9	6.1	2.5	90.5	100
207 (A1G)--V	7.389	4.1	0.5	1.9	93.5	100
208 (B2G)--V	7.954	0	0.9	5.5	93.6	100
209 (B1G)--V	8.031	0	0.5	0.1	99.5	100
210 (EU)--V	8.277	0.4	2	12.9	84.7	100
211 (EU)--V	8.277	0.4	2	12.9	84.7	100
212 (A1G)--V	8.534	0.2	1.6	2.1	96	100
213 (EU)--V	8.552	1.6	4.8	2.5	91	100
214 (EU)--V	8.552	1.6	4.8	2.5	91	100
215 (B2G)--V	8.835	0	5	23.5	71.5	100

216 B1G)--V	9.052	0	3.7	0.1	96.2	100
217 (B2G)--V	9.428	0	0.5	14.7	84.7	100
218 (A2G)--V	9.614	0	6.9	8.6	84.6	100
219 (EU)--V	9.79	2.8	3.8	17.7	75.6	100
220 (EU)--V	9.79	2.8	3.8	17.7	75.6	100
221 A1G)--V	9.813	1	16	13.3	69.7	100
222 (A2G)--V	10.494	0	0	0.6	99.4	100
223 (EU)--V	10.548	3.1	11.6	7.1	78.3	100
224 (EU)--V	10.548	3.1	11.6	7.1	78.3	100
225 (EU)--V	10.63	0.8	1.4	4.1	93.8	100
226 (EU)--V	10.63	0.8	1.4	4.1	93.8	100
227 (B1G)--V	10.869	0	19.3	7.7	73	100
228 (EU)--V	12.391	2.1	4.1	3.9	90	100
229 (EU)--V	12.391	2.1	4.1	3.9	90	100
230 (A2G)--V	12.521	0	0.3	6.6	93.1	100
231 (EG)--V	12.709	0	1.5	1.4	97.1	100
232 (EG)--V	12.709	0	1.5	1.4	97.1	100
233 (B2G)--V	12.722	0	0.3	0.1	99.6	100
234 (B2U)--V	12.921	0	0.4	0	99.6	100
235 (A2U)--V	13.029	3.8	0.2	0.7	95.4	100
236 (EU)--V	13.457	0.2	0.3	2.8	96.7	100
237 (EU)--V	13.457	0.2	0.3	2.8	96.7	100
238 (EG)--V	13.565	0	2.2	1.6	96.2	100
239 (EG)--V	13.565	0	2.2	1.6	96.2	100
240 (A2G)--V	13.823	0	0.7	2.1	97.2	100
241 A1G)--V	13.843	0.7	3.9	0.9	94.5	100
242 (B1U)--V	13.851	0	0	4.4	95.6	100
243 (B2G)--V	14.033	0	0.4	1.1	98.4	100
244 (EU)--V	14.191	0.1	0.4	0.6	98.9	100
245 (EU)--V	14.191	0.1	0.4	0.6	98.9	100
246 B1G)--V	14.199	0	34	5.1	60.9	100
247 (B2U)--V	14.381	0	1.3	0.1	98.6	100
248 (B2G)--V	14.441	0	0.8	1.8	97.4	100
249 (EU)--V	14.446	0	1.6	2.8	95.5	100
250 (EU)--V	14.446	0	1.6	2.8	95.5	100
251 A2U)--V	14.499	10.2	1.4	1.4	86.9	100
252 (A2G)--V	14.53	0	0.3	1	98.7	100
253 (B1G)--V	14.534	0	3.5	2	94.5	100
254 (EG)--V	14.665	0	0.5	1.6	97.9	100
255 (EG)--V	14.665	0	0.5	1.6	97.9	100
256 A1G)--V	14.702	1.8	1.5	16.6	80.2	100
257 (A1U)--V	14.806	0	0	0	100	100
258 (EU)--V	14.89	0.1	1.4	2.5	96	100
259 (EU)--V	14.89	0.1	1.4	2.5	96	100
260 (B1G)--V	14.967	0	25.7	1.6	72.7	100
261 A1G)--V	15.409	0.7	0.5	13.7	85.1	100
262 (EU)--V	15.418	0.1	12.1	17.3	70.4	100
263 (EU)--V	15.418	0.1	12.1	17.3	70.4	100
264 (A2G)--V	15.559	0	0.8	1.2	98	100
265 (B1U)--V	15.604	0	0	1.1	98.9	100
266 B1G)--V	15.607	0	3.2	0.3	96.5	100

267 (EU)--V	15.614	0.1	0.9	0.4	98.5	100
268 (EU)--V	15.614	0.1	0.9	0.4	98.5	100
269 (B2G)--V	15.662	0	0.9	11.8	87.3	100
270 (A1G)--V	15.732	2.2	6.6	5.1	86	100
271 (EG)--V	15.812	0	3.7	0.5	95.7	100
272 (EG)--V	15.812	0	3.7	0.5	95.7	100
273 (A1G)--V	16.062	0.5	23	12.5	64	100
274 (A2G)--V	16.111	0	0.8	2.9	96.2	100
275 (EU)--V	16.121	0.9	20.9	14	64.2	100
276 (EU)--V	16.121	0.9	20.9	14	64.2	100
277 (EU)--V	16.398	0.2	0.9	11.8	87.1	100
278 (EU)--V	16.398	0.2	0.9	11.8	87.1	100
279 (EU)--V	16.447	2.3	3.2	4	90.4	100
280 (EU)--V	16.447	2.3	3.2	4	90.4	100
281 (EG)--V	16.482	0	1.2	3.5	95.3	100
282 (EG)--V	16.482	0	1.2	3.5	95.3	100
283 (A2U)--V	16.524	3	1.1	1.3	94.6	100
284 (B2G)--V	16.543	0	0.8	13.7	85.6	100
285 (B2U)--V	16.618	0	1.7	0	98.3	100
286 A1U)--V	16.691	0	0	0	100	100
287 (B1G)--V	16.793	0.1	14.6	7.3	78.1	100
288 (B1U)--V	17.388	0	0	2.2	97.8	100
289 (EG)--V	17.511	0	0.6	0.3	99.1	100
290 (EG)--V	17.511	0	0.6	0.3	99.1	100
291 A2U)--V	17.713	0.7	0.4	4	94.9	100
292 (A1G)--V	17.956	5.9	22.8	4.1	67.2	100
293 (B2U)--V	18.986	0	1.1	0	98.9	100
294 (EG)--V	18.992	0	1.6	1.8	96.6	100
295 (EG)--V	18.992	0	1.6	1.8	96.6	100
296 A1U)--V	19.19	0	0	0	100	100
297 (EU)--V	19.464	5.5	16	6.9	71.7	100
298 (EU)--V	19.464	5.5	16	6.9	71.7	100
299 (B1U)--V	19.758	0	0	3.4	96.6	100
300 (EG)--V	20.223	0.3	36.2	6.9	56.6	100
301 (EG)--V	20.223	0.3	36.2	6.9	56.6	100
302 (B2G)--V	20.261	0	0.1	2.9	97	100
303 (EU)--V	20.457	0.1	1	1.4	97.6	100
304 (EU)--V	20.457	0.1	1	1.4	97.6	100
305 (A1G)--V	20.598	0.1	0.2	0.6	99.1	100
306 B2G)--V	20.937	0	1.6	1.8	96.6	100
307 (A2U)--V	20.983	1.2	12.2	55.6	31	100
308 (A2G)--V	21.125	0	0.2	0.5	99.2	100
309 (EU)--V	21.211	0.1	0.1	1.2	98.6	100
310 (EU)--V	21.211	0.1	0.1	1.2	98.6	100
311 (EG)--V	21.36	0	1.8	0.4	97.8	100
312 (EG)--V	21.36	0	1.8	0.4	97.8	100
313 (A2G)--V	21.565	0	1.4	1.2	97.3	100
314 (EU)--V	21.639	0	0.8	0.5	98.7	100
315 (EU)--V	21.639	0	0.8	0.5	98.7	100
316 B1G)--V	21.675	0	0.7	0.3	99	100
317 (B2G)--V	21.989	0	12.1	8.9	79	100

318 (A1G)--V	22.381	0.4	8.3	7.2	84	100
319 (B2G)--V	22.417	0	0.3	6.7	93	100
320 (EU)--V	22.534	0.2	1.7	3.3	94.8	100
321 (EU)--V	22.534	0.2	1.7	3.3	94.8	100
322 (B2U)--V	22.773	0	67.9	0	32	100
323 (A2G)--V	22.821	0	0.8	10.3	88.9	100
324 (A1U)--V	22.928	0	0	0	100	100
325 (B1G)--V	22.994	0	0.2	0.2	99.6	100
326 (EU)--V	23.001	0.1	0.4	3.3	96.2	100
327 (EU)--V	23.001	0.1	0.4	3.3	96.2	100
328 (A1G)--V	23.283	2.2	2.2	25.8	69.8	100
329 (EG)--V	23.548	0.1	14.4	41.1	44.3	100
330 (EG)--V	23.548	0.1	14.4	41.1	44.3	100
331 B1U)--V	23.576	0	0	63.7	36.3	100
332 (B1G)--V	23.9	0	20	9.9	70.1	100
333 (A1G)--V	23.941	0.9	10.6	7	81.5	100
334 (EU)--V	23.96	0.4	3.6	8.1	87.9	100
335 (EU)--V	23.96	0.4	3.6	8.1	87.9	100
336 (EU)--V	24.452	0.3	8.6	4.7	86.4	100
337 (EU)--V	24.452	0.3	8.6	4.7	86.4	100
338 (A2G)--V	24.574	0	0	0.1	99.9	100
339 (B1G)--V	24.717	0	0.2	0.3	99.5	100
340 (EU)--V	25.084	0.3	0.1	3.2	96.5	100
341 (EU)--V	25.084	0.3	0.1	3.2	96.5	100
342 (B2G)--V	25.511	0	0	0.6	99.4	100
343 (A2G)--V	25.594	0	0	1.8	98.2	100
344 (A2U)--V	25.635	4.6	42.7	16	36.8	100
345 (EU)--V	25.742	0	0.8	2.6	96.6	100
346 (EU)--V	25.742	0	0.8	2.6	96.6	100
347 (B2G)--V	26.198	0	1.3	2.3	96.3	100
348 (B1G)--V	26.419	0	8.6	1.9	89.5	100
349 (EU)--V	26.62	0.5	7.7	4.1	87.7	100
350 (EU)--V	26.62	0.5	7.7	4.1	87.7	100
351 A1G)--V	26.956	0	3.6	3.6	92.8	100
352 (EU)--V	26.979	0	6.4	5.9	87.7	100
353 (EU)--V	26.979	0	6.4	5.9	87.7	100
354 (A1G)--V	27.373	0.2	6	6.2	87.6	100
355 (B2G)--V	27.778	0	6.9	3.9	89.2	100
356 (EU)--V	28.212	0	2.2	2.8	95	100
357 (EU)--V	28.212	0	2.2	2.8	95	100
358 (A2G)--V	28.359	0	0.8	0.2	99	100
359 (A2G)--V	29.206	0	2.6	1.9	95.5	100
360 (B1G)--V	29.324	0	1.2	15.4	83.4	100
361 (EU)--V	29.483	0.1	1.1	0.7	98.1	100
362 (EU)--V	29.483	0.1	1.1	0.7	98.1	100
363 (B2G)--V	29.571	0	0.6	4.6	94.7	100
364 (B1G)--V	29.881	0	5.2	12.3	82.4	100
365 (A1G)--V	30.136	1	6.6	3.8	88.6	100
366 (EU)--V	30.281	0.2	5.7	3	91.1	100
367 (EU)--V	30.281	0.2	5.7	3	91.1	100
368 (B2G)--V	30.625	0	1.1	3.5	95.4	100



369 (A1G)--V	31.368	5.3	3.6	0.3	90.8	100
370 (EU)--V	31.514	1	6.5	4.7	87.8	100
371 (EU)--V	31.514	1	6.5	4.7	87.8	100
372 (B2U)--V	31.665	0	7.8	8.2	84	100
373 (A2G)--V	31.733	0	1.6	14	84.4	100
374 (EG)--V	32.043	0.2	5.3	14	80.5	100
375 (EG)--V	32.043	0.2	5.3	14	80.5	100
376 B1G)--V	32.328	0.3	10.7	8.8	80.2	100
377 (A2U)--V	32.644	0.2	0.8	10.4	88.5	100
378 (EU)--V	32.721	0.2	3.7	9.1	87	100
379 (EU)--V	32.721	0.2	3.7	9.1	87	100
380 (B2G)--V	32.962	0	1.7	1.9	96.3	100
381 (EG)--V	33.582	0	8.8	10.1	81.1	100
382 (EG)--V	33.582	0	8.8	10.1	81.1	100
383 (A1U)--V	33.583	0	20.3	18.4	61.4	100
384 (B2U)--V	33.66	0	6.3	10	83.7	100
385 (EU)--V	33.799	0.2	1.7	12.8	85.2	100
386 (EU)--V	33.799	0.2	1.7	12.8	85.2	100
387 (A2G)--V	34.172	0	0.7	8.2	91.1	100
388 (B1U)--V	34.558	0	5.2	6.5	88.3	100
389 (B1G)--V	34.599	0	0.4	4.3	95.3	100
390 (EG)--V	34.65	0.2	5.3	7	87.5	100
391 (EG)--V	34.65	0.2	5.3	7	87.5	100
392 (A1U)--V	34.882	0	3.6	5.7	90.7	100
393 (A1G)--V	35.24	3.3	5.4	0.1	91.1	100
394 (A2U)--V	35.364	4.2	26.6	17.5	51.8	100
395 (EU)--V	35.384	0.1	3.8	0.6	95.5	100
396 (EU)--V	35.384	0.1	3.8	0.6	95.5	100
397 (B1G)--V	35.451	0	6	0.2	93.8	100
398 (EG)--V	35.51	2.2	18.6	7.8	71.4	100
399 (EG)--V	35.51	2.2	18.6	7.8	71.4	100
400 (EU)--V	36.313	0.3	6.7	0.2	92.8	100
401 (EU)--V	36.313	0.3	6.7	0.2	92.8	100
402 (B2U)--V	37.13	0	28.4	0.7	70.9	100
403 (A1G)--V	37.253	0.1	0.4	0	99.5	100
404 (EU)--V	37.508	0.1	1.3	1.5	97.2	100
405 (EU)--V	37.508	0.1	1.3	1.5	97.2	100
406 A2G)--V	37.559	0	3.1	17.3	79.6	100
407 (B1G)--V	37.567	0	0.1	1.1	98.8	100
408 (B2G)--V	37.589	0	0.1	0.4	99.5	100
409 (EG)--V	37.886	0.2	3.8	5.8	90.2	100
410 (EG)--V	37.886	0.2	3.8	5.8	90.2	100
411 A2U)--V	37.901	0.6	2.1	1.8	95.5	100
412 (B2U)--V	37.976	0	0.2	0.7	99.1	100
413 (EG)--V	38.236	0.5	12.3	12	75.3	100
414 (EG)--V	38.236	0.5	12.3	12	75.3	100
415 (A2U)--V	38.447	2.2	9.7	0.7	87.3	100
416 B2U)--V	38.79	0	2.3	0.7	97	100
417 (B1U)--V	38.827	0	17.9	23.1	59	100
418 (EG)--V	39.059	0.3	6	3.1	90.6	100
419 (EG)--V	39.059	0.3	6	3.1	90.6	100

420 (A1U)--V	39.097	0	0	0	100	100
421 B1U)--V	39.162	0	4.8	6.7	88.5	100
422 (EG)--V	39.182	0.6	14.1	8.7	76.7	100
423 (EG)--V	39.182	0.6	14.1	8.7	76.7	100
424 (EU)--V	39.199	0	1.3	0.7	98	100
425 (EU)--V	39.199	0	1.3	0.7	98	100
426 A2G)--V	39.833	0	4.4	0.1	95.6	100
427 (A2U)--V	40.026	7.8	39.3	6.2	46.7	100
428 (A2G)--V	40.805	0	2.1	4.2	93.7	100
429 (B2G)--V	41.556	0	0.1	1.5	98.5	100
430 (EU)--V	41.653	0.2	4.4	0.1	95.2	100
431 (EU)--V	41.653	0.2	4.4	0.1	95.2	100
432 (A1G)--V	41.957	0.1	40.8	0.8	58.4	100
433 (EU)--V	42.236	0.8	13	2.6	83.5	100
434 (EU)--V	42.236	0.8	13	2.6	83.5	100
435 (A1G)--V	43.22	0.4	42.3	1.3	56	100
436 B1G)--V	43.673	0	33	2.7	64.3	100
437 (B2G)--V	44.743	0	0.2	19.6	80.2	100
438 (EU)--V	45.284	0.7	0.8	43.7	54.7	100
439 (EU)--V	45.284	0.7	0.8	43.7	54.7	100
440 (A1G)--V	45.532	1	0.8	53.6	44.6	100
441 B1G)--V	46.019	0	44.1	10.5	45.4	100
442 (EU)--V	46.345	0.2	35.6	4.2	60	100
443 (EU)--V	46.345	0.2	35.6	4.2	60	100
444 (B1U)--V	46.448	0	1.5	12.4	86.1	100
445 (A1G)--V	46.513	0.6	44.9	3.5	51.1	100
446 (EG)--V	46.762	0	2.5	10	87.6	100
447 (EG)--V	46.762	0	2.5	10	87.6	100
448 (A1U)--V	47.227	0	3.6	2.7	93.7	100
449 (B1G)--V	47.609	0	53.5	1.6	44.9	100
450 (B2G)--V	48.013	0	0.1	10.1	89.7	100
451 (EU)--V	48.052	0.1	21.4	2.4	76.2	100
452 (EU)--V	48.052	0.1	21.4	2.4	76.2	100
453 (A1G)--V	48.219	0.1	22.3	2	75.7	100
454 (EU)--V	48.382	0.1	1.1	22.4	76.4	100
455 (EU)--V	48.382	0.1	1.1	22.4	76.4	100
456 A2G)--V	48.433	0	0.5	0	99.5	100
457 (A2U)--V	48.601	0.5	10.6	25.1	63.9	100
458 (A1G)--V	48.914	0.6	18.6	41.3	39.5	100
459 (EU)--V	49.359	0.1	9.8	1.3	88.8	100
460 (EU)--V	49.359	0.1	9.8	1.3	88.8	100
461 B1G)--V	49.38	0	31.2	5.2	63.6	100
462 (EG)--V	49.656	0.5	16.1	17.5	66	100
463 (EG)--V	49.656	0.5	16.1	17.5	66	100
464 (A2G)--V	49.787	0	0	0	99.9	100
465 (B2G)--V	50.164	0	0	0.9	99.1	100
466 (EU)--V	50.245	0	0.4	0.8	98.7	100
467 (EU)--V	50.245	0	0.4	0.8	98.7	100
468 (A1G)--V	50.321	0	10.6	39.5	49.8	100
469 (EU)--V	50.632	2.2	6.1	22.9	68.9	100
470 (EU)--V	50.632	2.2	6.1	22.9	68.9	100

471 B2U)--V	50.695	0	26.3	11.6	62	100
472 (B1G)--V	50.804	0	7.6	2.4	89.9	100
473 (B1G)--V	50.875	0	14.4	5.4	80.2	100
474 (EU)--V	51.161	3.6	13.7	9.5	73.2	100
475 (EU)--V	51.161	3.6	13.7	9.5	73.2	100
476 (EU)--V	51.725	13	30.7	0.6	55.7	100
477 (EU)--V	51.725	13	30.7	0.6	55.7	100
478 (A1G)--V	52.145	0.6	7.1	13.1	79.2	100
479 (A2G)--V	52.198	0	0	0.7	99.3	100
480 (B2G)--V	52.596	0	0.3	8.5	91.2	100
481 B2U)--V	52.958	0	26.6	14.3	59.1	100
482 (EU)--V	53.003	0	3.5	1.3	95.2	100
483 (EU)--V	53.003	0	3.5	1.3	95.2	100
484 (A1G)--V	53.733	0	18.2	14.2	67.5	100
485 (EU)--V	53.768	0.1	6.1	3.6	90.2	100
486 (EU)--V	53.768	0.1	6.1	3.6	90.2	100
487 (EG)--V	54.15	1.4	28.3	17	53.3	100
488 (EG)--V	54.15	1.4	28.3	17	53.3	100
489 (B1G)--V	54.182	0	28.3	3.9	67.8	100
490 (A2G)--V	55.236	0	8.3	4.6	87.1	100
491 B1U)--V	55.292	0	2.5	28.9	68.5	100
492 (A1U)--V	55.337	0	24.8	11.3	63.9	100
493 (EG)--V	55.341	5.1	4.7	20.1	70.1	100
494 (EG)--V	55.341	5.1	4.7	20.1	70.1	100
495 (A2U)--V	55.393	0.3	4.9	20.7	74	100
496 B2G)--V	55.441	0	0.2	0.3	99.5	100
497 (EU)--V	55.694	0.1	0.8	1.3	97.7	100
498 (EU)--V	55.694	0.1	0.8	1.3	97.7	100
499 (A2G)--V	55.862	0	2.5	2.6	94.9	100
500 (EU)--V	56.084	0	2.4	4.7	92.9	100
501 (EU)--V	56.084	0	2.4	4.7	92.9	100
502 (B1G)--V	56.615	0	5	9.4	85.6	100
503 (B2G)--V	56.754	0	0.3	6.1	93.6	100
504 (EU)--V	56.987	0	0.7	3.3	95.9	100
505 (EU)--V	56.987	0	0.7	3.3	95.9	100
506 (EG)--V	57.147	57.1	14.1	0.8	28	100
507 (EG)--V	57.147	57.1	14.1	0.8	28	100
508 (A1G)--V	57.242	0.7	4.4	0.8	94.1	100
509 (B1U)--V	57.955	0	9.6	13.4	77	100
510 (EG)--V	57.971	16.1	9.2	5.2	69.5	100
511 (EG)--V	57.971	16.1	9.2	5.2	69.5	100
512 (A1U)--V	58.795	0	5.4	4.8	89.7	100
513 (B2U)--V	58.923	0	1.1	0	98.9	100
514 (A2G)--V	58.953	0	0.1	0.3	99.7	100
515 (EU)--V	59.134	0	3.8	6.6	89.5	100
516 (EU)--V	59.134	0	3.8	6.6	89.5	100
517 (EG)--V	59.47	0.1	9	0.1	90.8	100
518 (EG)--V	59.47	0.1	9	0.1	90.8	100
519 (B1U)--V	59.575	0	6.5	1.4	92.1	100
520 (EG)--V	59.746	1.3	1.3	6.3	91.1	100
521 (EG)--V	59.746	1.3	1.3	6.3	91.1	100

522 (A2U)--V	59.864	0.2	25.3	6.5	68	100
523 (A2U)--V	59.949	0.1	19.4	0.4	80.2	100
524 (B2G)--V	60.063	0	0.2	11.8	88	100
525 (A1U)--V	60.074	0	0.2	4.8	95	100
526 A2G)--V	60.084	0	3.3	1.4	95.3	100
527 (EU)--V	60.57	2.1	13.4	16.2	68.2	100
528 (EU)--V	60.57	2.1	13.4	16.2	68.2	100
529 (B1G)--V	60.803	0	36.4	16.5	47	100
530 (B2U)--V	60.979	0	2.5	1.2	96.4	100
531 (EG)--V	60.99	0	8.6	4.4	87	100
532 (EG)--V	60.99	0	8.6	4.4	87	100
533 (A1G)--V	61.834	0.1	1.2	17.6	81.2	100
534 (B2G)--V	62.018	5.6	6.2	2.8	85.4	100
535 (B1U)--V	62.788	0	18.1	1.8	80.1	100
536 (EU)--V	63.236	0.1	1.8	25.7	72.3	100
537 (EU)--V	63.236	0.1	1.8	25.7	72.3	100
538 (EG)--V	63.84	0.6	15.3	8.8	75.3	100
539 (EG)--V	63.84	0.6	15.3	8.8	75.3	100
540 (A2G)--V	63.846	0	0.1	0	99.9	100
541 (EU)--V	64.237	0	0.2	0.5	99.2	100
542 (EU)--V	64.237	0	0.2	0.5	99.2	100
543 (B2G)--V	64.503	0	2.7	25.8	71.5	100
544 (B1G)--V	64.558	0	1.7	0.1	98.2	100
545 (B2G)--V	64.999	0.3	2.7	1.8	95.3	100
546 A1G)--V	65.989	2.3	16.9	1.8	79	100
547 (A1U)--V	66.021	0	2.6	6.7	90.7	100
548 (A2U)--V	66.172	0.1	8.7	19.2	72	100
549 (EU)--V	66.318	0.2	8.8	11.1	79.9	100
550 (EU)--V	66.318	0.2	8.8	11.1	79.9	100
551 (EG)--V	67.235	0	7.6	10	82.5	100
552 (EG)--V	67.235	0	7.6	10	82.5	100
553 (A1U)--V	68.322	0	13.5	12.3	74.3	100
554 (B1U)--V	68.434	0	12.3	8.3	79.5	100
555 (B1G)--V	69.355	0.7	56.8	4.8	37.6	100
556 A1G)--V	69.489	2.9	17.7	35.7	43.7	100
557 (A2G)--V	69.844	0	0.7	0.3	99	100
558 (EG)--V	70.217	0.3	7.1	10.7	81.8	100
559 (EG)--V	70.217	0.3	7.1	10.7	81.8	100
560 (EU)--V	70.223	0	0.3	0.5	99.2	100
561 (EU)--V	70.223	0	0.3	0.5	99.2	100
562 (B2G)--V	70.232	0	0.3	0.1	99.6	100
563 (EU)--V	70.44	0.1	16.5	10.8	72.6	100
564 (EU)--V	70.44	0.1	16.5	10.8	72.6	100
565 (B1G)--V	70.662	0	0.5	3.6	95.8	100
566 (EU)--V	70.846	0.1	26.5	26.5	46.8	100
567 (EU)--V	70.846	0.1	26.5	26.5	46.8	100
568 (A1G)--V	70.884	2.9	11.4	24.1	61.6	100
569 (A2G)--V	71.019	0	2.2	1.7	96.1	100
570 (B1U)--V	71.056	0	0.2	4.2	95.7	100
571 (EU)--V	71.199	0	9.9	8.2	81.9	100
572 (EU)--V	71.199	0	9.9	8.2	81.9	100

573 (B1G)--V	71.365	0	27.6	3.7	68.7	100
574 (A1G)--V	71.692	5.2	6.4	0.4	88	100
575 (B2U)--V	72.184	0	15.9	30.8	53.3	100
576 A1U)--V	72.33	0	5.5	16.8	77.6	100
577 (B1G)--V	72.331	0.2	25.7	3.8	70.3	100
578 (EG)--V	72.38	0.2	10	22.2	67.6	100
579 (EG)--V	72.38	0.2	10	22.2	67.6	100
580 (EU)--V	72.413	0.1	40.5	14.2	45.2	100
581 (EU)--V	72.413	0.1	40.5	14.2	45.2	100
582 (A1G)--V	72.633	0.1	53.8	20.4	25.7	100
583 (B2G)--V	73.395	0	0.2	7	92.8	100
584 (B2G)--V	73.756	0.1	3.9	21.4	74.6	100
585 (EU)--V	74.126	0	2.1	6.5	91.3	100
586 (EU)--V	74.126	0	2.1	6.5	91.3	100
587 (A2G)--V	74.472	0	0.9	6.6	92.5	100
588 (B1G)--V	74.498	1.2	52.9	4.6	41.2	100
589 (B2G)--V	74.974	0	0.1	0.2	99.7	100
590 (EU)--V	75.702	0	2.6	4.6	92.8	100
591 (EU)--V	75.702	0	2.6	4.6	92.8	100
592 (EU)--V	77.286	0.1	7.3	4.7	87.9	100
593 (EU)--V	77.286	0.1	7.3	4.7	87.9	100
594 (A2G)--V	77.416	0	1.2	2.6	96.2	100
595 (A1G)--V	77.728	0.2	21.3	25.2	53.4	100
596 (EU)--V	77.817	0.4	6.3	5.5	87.9	100
597 (EU)--V	77.817	0.4	6.3	5.5	87.9	100
598 (B2G)--V	79.324	0	0.1	7.8	92.1	100
599 (B1G)--V	79.34	0.8	6.5	5.9	86.8	100
600 (A2G)--V	80.337	0	0.4	0	99.6	100
601 A1G)--V	80.774	0.4	4	5.1	90.5	100
602 (EU)--V	80.904	0.1	9.8	10.9	79.3	100
603 (EU)--V	80.904	0.1	9.8	10.9	79.3	100
604 (A2G)--V	81.581	0	14.9	4.4	80.6	100
605 (B2G)--V	82.786	0	2.3	2.5	95.2	100
606 (EU)--V	83.263	0	1	5.1	93.9	100
607 (EU)--V	83.263	0	1	5.1	93.9	100
608 (EU)--V	85.662	0.2	7.4	19.7	72.7	100
609 (EU)--V	85.662	0.2	7.4	19.7	72.7	100
610 (B1G)--V	86.96	0.8	5.2	25.7	68.4	100
611 A1G)--V	88.893	0.4	4.3	54.9	40.4	100
612 (B2G)--V	89.35	0	1	1.8	97.2	100
613 (EU)--V	90.526	0	1.5	3	95.6	100
614 (EU)--V	90.526	0	1.5	3	95.6	100
615 (A2G)--V	91.227	0	7.5	12.8	79.8	100
616 A2G)--V	91.335	0	1.8	1.5	96.8	100
617 (EU)--V	93.258	0	5.5	4.4	90	100
618 (EU)--V	93.258	0	5.5	4.4	90	100
619 (B2G)--V	93.932	0	4	3	93	100

## BP86 Exchange Correlation Functional

Orbital	Index	Energy,eV	1	2	3	4	5
	1 A1G)--O	-9409.89	100	0	0	0	100
	2 (A1G)--O	-1134.22	100	0	0	0	100
	3 (A2U)--O	-1000.25	100	0	0	0	100
	4 (EU)--O	-1000.06	100	0	0	0	100
	5 (EU)--O	-1000.06	100	0	0	0	100
	6 (EU)--O	-381.955	0	99.8	0	0.2	100
	7 (EU)--O	-381.955	0	99.8	0	0.2	100
	8 (B1G)--O	-381.955	0	99.7	0	0.2	100
	9 (A1G)--O	-381.955	0	99.9	0	0.1	100
	10 (B2G)--O	-381.646	0	0	99.7	0.3	100
	11 (EU)--O	-381.646	0	0	99.7	0.3	100
	12 (EU)--O	-381.646	0	0	99.7	0.3	100
	13 (A1G)--O	-381.646	0	0	99.8	0.2	100
	14 (B2G)--O	-271.721	0	0	0.2	99.8	100
	15 (EU)--O	-271.721	0	0	0.1	99.9	100
	16 (EU)--O	-271.721	0	0	0.1	99.9	100
	17 (A1G)--O	-271.72	0	0	0	100	100
	18 (A2G)--O	-271.72	0	0	0	100	100
	19 (EU)--O	-271.719	0	0	0	100	100
	20 (EU)--O	-271.719	0	0	0	100	100
	21 B1G)--O	-271.719	0	0	0	100	100
	22 (EU)--O	-269.961	0	0	0	100	100
	23 (EU)--O	-269.961	0	0	0	100	100
	24 (A1G)--O	-269.961	0	0	0	100	100
	25 (B1G)--O	-269.961	0	0	0	100	100
	26 A2G)--O	-269.956	0	0	0	100	100
	27 (EU)--O	-269.956	0	0	0	100	100
	28 (EU)--O	-269.956	0	0	0	100	100
	29 (B2G)--O	-269.956	0	0	0	100	100
	30 (B1G)--O	-269.949	0	0	0	100	100
	31 (EU)--O	-269.949	0	0	0	100	100
	32 (EU)--O	-269.949	0	0	0	100	100
	33 (A1G)--O	-269.949	0	0	0	100	100
	34 (A2G)--O	-269.948	0	0	0	100	100
	35 (EU)--O	-269.948	0	0	0	100	100
	36 (EU)--O	-269.948	0	0	0	100	100
	37 (B2G)--O	-269.948	0	0	0	100	100
	38 (B1G)--O	-269.939	0	0	0	100	100
	39 (EU)--O	-269.939	0	0	0	100	100
	40 (EU)--O	-269.939	0	0	0	100	100
	41 A1G)--O	-269.939	0	0	0	100	100
	42 (A2G)--O	-269.934	0	0	0	100	100
	43 (EU)--O	-269.934	0	0	0	100	100
	44 (EU)--O	-269.934	0	0	0	100	100

45 (B2G)--O	-269.934	0	0	0	100	100
46 A1G)--O	-125.051	100	0	0	0	100
47 (A2U)--O	-82.615	100	0	0	0	100
48 (EU)--O	-82.299	100	0	0	0	100
49 (EU)--O	-82.299	100	0	0	0	100
50 (A1G)--O	-25.203	0.4	39.9	25.1	34.6	100
51 (EU)--O	-24.835	0.2	39.1	24.7	36	100
52 (EU)--O	-24.835	0.2	39.1	24.7	36	100
53 (B1G)--O	-24.122	0.1	59.3	0.8	39.8	100
54 (B2G)--O	-23.551	0	1.8	69.9	28.3	100
55 (EU)--O	-22.502	0	17.8	50.3	31.8	100
56 (EU)--O	-22.502	0	17.8	50.3	31.8	100
57 (A1G)--O	-21.697	0.1	17.1	50.2	32.5	100
58 (A1G)--O	-21.242	0.4	21.4	7.7	70.5	100
59 (EU)--O	-21.224	0.1	14.5	1.2	84.3	100
60 (EU)--O	-21.224	0.1	14.5	1.2	84.3	100
61 B1G)--O	-21.21	0.1	13	0	86.9	100
62 (A2G)--O	-19.179	0	2.9	6.8	90.3	100
63 (A1G)--O	-18.861	0.7	12.7	0.3	86.3	100
64 (EU)--O	-18.831	0.1	14	4.2	81.8	100
65 (EU)--O	-18.831	0.1	14	4.2	81.8	100
66 (EU)--O	-18.718	0	4.4	1.3	94.2	100
67 (EU)--O	-18.718	0	4.4	1.3	94.2	100
68 (B1G)--O	-18.707	0.4	19.3	0.7	79.7	100
69 (B2G)--O	-18.639	0	0	1.8	98.2	100
70 (A2G)--O	-17.824	0	5.5	8.4	86	100
71 (EU)--O	-17.169	0	7	18.4	74.7	100
72 (EU)--O	-17.169	0	7	18.4	74.7	100
73 (B1G)--O	-15.816	0.7	11.3	20.3	67.7	100
74 (A1G)--O	-15.701	2.1	11.7	0.5	85.8	100
75 (EU)--O	-15.534	0.2	11.2	0.4	88.1	100
76 (EU)--O	-15.534	0.2	11.2	0.4	88.1	100
77 (B2G)--O	-15.375	0	3.1	13.9	82.9	100
78 (B1G)--O	-15.291	0.6	5.8	9.6	84.1	100
79 (EU)--O	-14.658	0	6.1	3.2	90.6	100
80 (EU)--O	-14.658	0	6.1	3.2	90.6	100
81 B2G)--O	-14.594	1.5	31	22.9	44.6	100
82 (A2G)--O	-14.416	0	5.9	1.5	92.6	100
83 (A1G)--O	-13.666	3.1	8.1	1.4	87.4	100
84 (EU)--O	-13.514	0	18.5	14	67.5	100
85 (EU)--O	-13.514	0	18.5	14	67.5	100
86 (EU)--O	-13.115	0.4	13.4	18.2	68.1	100
87 (EU)--O	-13.115	0.4	13.4	18.2	68.1	100
88 (B1G)--O	-13.071	5.4	12.5	5.5	76.6	100
89 (A2G)--O	-12.317	0	24.1	14.7	61.2	100
90 (B2G)--O	-12.236	0.9	2	1.6	95.5	100
91 A1G)--O	-11.874	19.3	20.9	1.4	58.4	100
92 (EU)--O	-11.754	0	2.5	4	93.4	100

93 (EU)--O	-11.754	0	2.5	4	93.4	100
94 (B1G)--O	-11.661	31.1	19.2	0.2	49.5	100
95 (A2U)--O	-11.383	0.5	25.3	17.9	56.4	100
96 (EU)--O	-11.337	0.7	13.7	1.2	84.5	100
97 (EU)--O	-11.337	0.7	13.7	1.2	84.5	100
98 (A2G)--O	-11.253	0	0.6	7.1	92.4	100
99 (EG)--O	-11.093	17.8	24.9	12.3	45	100
100 (EG)--O	-11.093	17.8	24.9	12.3	45	100
101 A1G)--O	-10.822	7	8.2	5.7	79.1	100
102 (B1G)--O	-10.755	23.4	10.8	1.8	64	100
103 (EU)--O	-10.682	0	1.2	1.4	97.4	100
104 (EU)--O	-10.682	0	1.2	1.4	97.4	100
105 (B2G)--O	-10.678	0.3	0.1	0.7	98.9	100
106 A1G)--O	-10.429	43.3	5.9	2.2	48.5	100
107 (A2G)--O	-10.409	0	0.6	3.9	95.4	100
108 (EU)--O	-10.315	0.3	5.3	4.4	90	100
109 (EU)--O	-10.315	0.3	5.3	4.4	90	100
110 (B2U)--O	-10.267	0	26.5	0	73.5	100
111 (EG)--O	-10.015	88.4	1.2	1.9	8.5	100
112 (EG)--O	-10.015	88.4	1.2	1.9	8.5	100
113 (B2G)--O	-9.921	49.2	6.3	0.9	43.6	100
114 (B1G)--O	-9.916	17.6	1.3	3.1	78	100
115 (B1U)--O	-9.405	0	0.1	50.6	49.4	100
116 A1G)--O	-9.4	63.9	11.5	2.4	22.2	100
117 (B2G)--O	-8.907	1.5	0.2	1.6	96.8	100
118 (EG)--O	-8.882	2.4	1.9	15.2	80.5	100
119 (EG)--O	-8.882	2.4	1.9	15.2	80.5	100
120 (A2U)--O	-8.861	0.3	7.1	4	88.6	100
121 (EU)--O	-8.836	0	1.6	1.9	96.5	100
122 (EU)--O	-8.836	0	1.6	1.9	96.5	100
123 (A2G)--O	-8.643	0	1.9	1.1	97	100
124 (EU)--O	-8.498	4.7	33.3	2.5	59.5	100
125 (EU)--O	-8.498	4.7	33.3	2.5	59.5	100
126 A1G)--O	-8.483	0	1.7	3	95.3	100
127 (B2U)--O	-8.478	0	25.6	0	74.3	100
128 (B1G)--O	-8.131	1.6	0.6	3	94.8	100
129 (EU)--O	-8.131	2.6	16.4	6.4	74.6	100
130 (EU)--O	-8.131	2.6	16.4	6.4	74.6	100
131 (EG)--O	-7.811	3.3	19.5	20	57.2	100
132 (EG)--O	-7.811	3.3	19.5	20	57.2	100
133 (A1G)--O	-7.041	0.2	19.2	53.3	27.2	100
134 (A1U)--O	-6.821	0	0	0	99.9	100
135 (A2U)--O	-6.387	3.2	48.1	24.6	24.1	100
136 (EU)--O	-6.359	0.2	18.1	49.8	31.9	100
137 (EU)--O	-6.359	0.2	18.1	49.8	31.9	100
138 (B1U)--O	-6.325	0	0	5.3	94.7	100
139 (EG)--O	-6.304	0	0.4	10.1	89.5	100
140 (EG)--O	-6.304	0	0.4	10.1	89.5	100



141 A2U)--O	-6.21	0.1	3.6	36.2	60.1	100
142 (EG)--O	-6.09	2.1	28.6	1.6	67.6	100
143 (EG)--O	-6.09	2.1	28.6	1.6	67.6	100
144 (B2U)--O	-6.078	0	26	0	74	100
145 (B2G)--O	-5.882	0.7	12.1	61.1	26.2	100
146 B1G)--O	-5.407	24.7	48.3	0.8	26.3	100
147 (A1U)--O	-4.746	0	0.1	0.1	99.8	100
148 (EG)--V	-3.291	0.4	13.3	19.8	66.5	100
149 (EG)--V	-3.291	0.4	13.3	19.8	66.5	100
150 (B1U)--V	-1.87	0	0	25.1	74.9	100
151 B2U)--V	-1.651	0	19.6	0	80.4	100
152 (A2U)--V	-1.52	5.8	1.2	5.6	87.5	100
153 (EG)--V	-1.382	0.1	5.6	3.6	90.6	100
154 (EG)--V	-1.382	0.1	5.6	3.6	90.6	100
155 (A1U)--V	-0.203	0	0	0	100	100
156 (EG)--V	-0.144	0	1.8	0.9	97.3	100
157 (EG)--V	-0.144	0	1.8	0.9	97.3	100
158 (A2U)--V	0.182	59.7	6.7	3.2	30.4	100
159 (B2U)--V	0.414	0	19.4	0.1	80.5	100
160 (A1G)--V	0.423	68.1	19.7	0.4	11.8	100
161 B1U)--V	0.611	0	0.1	18.6	81.4	100
162 (EG)--V	1.902	0.1	14.4	15.9	69.5	100
163 (EG)--V	1.902	0.1	14.4	15.9	69.5	100
164 (A1G)--V	1.925	0.2	0.1	2	97.7	100
165 (EU)--V	1.987	5.6	1.2	1.2	92	100
166 (EU)--V	1.987	5.6	1.2	1.2	92	100
167 (B1G)--V	2.112	0	0	0.1	99.9	100
168 (EU)--V	2.355	62	10	2.7	25.3	100
169 (EU)--V	2.355	62	10	2.7	25.3	100
170 (A2U)--V	2.663	25.6	18.3	16.7	39.5	100
171 B2G)--V	2.955	0	1.1	0.2	98.7	100
172 (EU)--V	3.141	0	1.2	0.2	98.6	100
173 (EU)--V	3.141	0	1.2	0.2	98.6	100
174 (A1G)--V	3.201	32.2	0.4	10.9	56.5	100
175 (A2G)--V	3.368	0	0.7	0	99.2	100
176 A1U)--V	3.544	0	0	0	100	100
177 (EG)--V	3.721	0	0.9	4.1	95	100
178 (EG)--V	3.721	0	0.9	4.1	95	100
179 (B1U)--V	3.739	0	0	4.6	95.4	100
180 (EU)--V	3.817	1.5	0.1	3.4	94.9	100
181 (EU)--V	3.817	1.5	0.1	3.4	94.9	100
182 (B2G)--V	3.832	0	0.1	5.6	94.3	100
183 (A1G)--V	4.118	33.8	0.9	0.3	64.9	100
184 (B1G)--V	4.163	0	6.2	0.3	93.5	100
185 (EU)--V	4.169	1.5	2.2	0.2	96.1	100
186 (EU)--V	4.169	1.5	2.2	0.2	96.1	100
187 (A2G)--V	4.364	0	0.1	0	99.8	100
188 (EU)--V	4.849	6.3	8.8	3.5	81.4	100

189 (EU)--V	4.849	6.3	8.8	3.5	81.4	100
190 (B2G)--V	4.863	0.1	3.2	9.9	86.8	100
191 B1G)--V	5.015	0	26.5	3.6	69.9	100
192 (A1G)--V	5.053	0	0.6	1.1	98.2	100
193 (EU)--V	5.551	0.3	0.6	2.1	97	100
194 (EU)--V	5.551	0.3	0.6	2.1	97	100
195 (A2U)--V	5.645	89.8	2.4	0.9	6.9	100
196 A2G)--V	5.696	0	6	0.6	93.4	100
197 (B2G)--V	5.922	0	0.3	12.3	87.4	100
198 (EU)--V	5.93	1	0.3	5.9	92.8	100
199 (EU)--V	5.93	1	0.3	5.9	92.8	100
200 (B1G)--V	6.24	0	2.4	0	97.5	100
201 A2G)--V	6.262	0	0.3	0	99.7	100
202 (A1G)--V	6.518	9.5	10.3	20.4	59.8	100
203 (EU)--V	6.608	1.7	6	2.4	89.9	100
204 (EU)--V	6.608	1.7	6	2.4	89.9	100
205 (EU)--V	6.94	1	6.1	2.7	90.2	100
206 (EU)--V	6.94	1	6.1	2.7	90.2	100
207 (A1G)--V	7.087	5.5	0.6	2.7	91.2	100
208 (B2G)--V	7.615	0	0.8	4.2	95	100
209 (B1G)--V	7.694	0	0.4	0.1	99.6	100
210 (EU)--V	7.972	0.4	2.1	12.7	84.8	100
211 (EU)--V	7.972	0.4	2.1	12.7	84.8	100
212 (A1G)--V	8.226	0.3	1.6	2.1	96.1	100
213 (EU)--V	8.242	1.8	4.6	1.9	91.7	100
214 (EU)--V	8.242	1.8	4.6	1.9	91.7	100
215 (B2G)--V	8.545	0	5.1	23.8	71.2	100
216 B1G)--V	8.78	0	3.6	0.1	96.3	100
217 (B2G)--V	9.06	0	0.6	14.5	84.9	100
218 (A2G)--V	9.305	0	7	8.4	84.6	100
219 (EU)--V	9.455	2.7	3.6	17.8	75.9	100
220 (EU)--V	9.455	2.7	3.6	17.8	75.9	100
221 A1G)--V	9.526	1	16	13.2	69.9	100
222 (A2G)--V	10.195	0	0	0.6	99.4	100
223 (EU)--V	10.257	3.2	11.8	6.9	78.1	100
224 (EU)--V	10.257	3.2	11.8	6.9	78.1	100
225 (EU)--V	10.335	0.7	1.3	3.9	94.1	100
226 (EU)--V	10.335	0.7	1.3	3.9	94.1	100
227 (B1G)--V	10.556	0	19.3	7.6	73.1	100
228 (EU)--V	12.107	2.1	4.2	4	89.7	100
229 (EU)--V	12.107	2.1	4.2	4	89.7	100
230 (A2G)--V	12.23	0	0.3	6.9	92.8	100
231 B2G)--V	12.478	0	0.3	0.1	99.6	100
232 (EG)--V	12.58	0	1.5	1.4	97.1	100
233 (EG)--V	12.58	0	1.5	1.4	97.1	100
234 (B2U)--V	12.788	0	0.4	0	99.6	100
235 (A2U)--V	12.897	3.9	0.1	0.7	95.3	100
236 (EU)--V	13.247	0.2	0.4	3	96.5	100

237 (EU)--V	13.247	0.2	0.4	3	96.5	100
238 (EG)--V	13.434	0	2.3	1.6	96.1	100
239 (EG)--V	13.434	0	2.3	1.6	96.1	100
240 (A1G)--V	13.518	0.7	3.4	0.8	95.1	100
241 A2G)--V	13.612	0	0.8	2.2	97	100
242 (B1U)--V	13.735	0	0	4.5	95.4	100
243 (B2G)--V	13.806	0	0.4	1.5	98.1	100
244 (B1G)--V	13.826	0	34	5.1	61	100
245 (EU)--V	13.937	0.1	0.4	0.4	99.1	100
246 (EU)--V	13.937	0.1	0.4	0.4	99.1	100
247 (EU)--V	14.153	0	0.7	1.6	97.7	100
248 (EU)--V	14.153	0	0.7	1.6	97.7	100
249 (B1G)--V	14.195	0	2.2	2.8	95	100
250 (B2G)--V	14.222	0	0.8	1.8	97.5	100
251 B2U)--V	14.256	0	1.3	0.1	98.6	100
252 (A2G)--V	14.343	0	0.3	0.9	98.8	100
253 (A2U)--V	14.383	10.6	1.4	1.4	86.6	100
254 (A1G)--V	14.451	1.9	1.5	15.3	81.3	100
255 (EG)--V	14.55	0	0.5	1.7	97.8	100
256 (EG)--V	14.55	0	0.5	1.7	97.8	100
257 (EU)--V	14.629	0.1	1.3	2	96.6	100
258 (EU)--V	14.629	0.1	1.3	2	96.6	100
259 (A1U)--V	14.695	0	0	0	100	100
260 (B1G)--V	14.715	0	25.7	1.2	73	100
261 A1G)--V	15.164	1	0.1	13.3	85.6	100
262 (EU)--V	15.192	0.2	13.7	16.5	69.5	100
263 (EU)--V	15.192	0.2	13.7	16.5	69.5	100
264 (A2G)--V	15.337	0	0.9	1.6	97.4	100
265 (B1G)--V	15.41	0	1.7	0.6	97.8	100
266 (EU)--V	15.415	0.2	0.8	0.3	98.8	100
267 (EU)--V	15.415	0.2	0.8	0.3	98.8	100
268 (B2G)--V	15.446	0	0.9	11.7	87.4	100
269 (B1U)--V	15.491	0	0	1.1	98.9	100
270 (A1G)--V	15.513	1.8	17.5	3.1	77.7	100
271 (EG)--V	15.691	0	4	0.5	95.4	100
272 (EG)--V	15.691	0	4	0.5	95.4	100
273 (A1G)--V	15.738	0.4	21.9	14.7	63.1	100
274 (EU)--V	15.828	1.2	21.8	11.9	65	100
275 (EU)--V	15.828	1.2	21.8	11.9	65	100
276 A2G)--V	15.872	0	0.8	2.9	96.2	100
277 (EU)--V	16.185	1.5	3.2	2.1	93.2	100
278 (EU)--V	16.185	1.5	3.2	2.1	93.2	100
279 (EU)--V	16.212	1.5	2	12.1	84.5	100
280 (EU)--V	16.212	1.5	2	12.1	84.5	100
281 B2G)--V	16.341	0	0.7	13.8	85.5	100
282 (EG)--V	16.368	0	1.3	3.7	95	100
283 (EG)--V	16.368	0	1.3	3.7	95	100
284 (A2U)--V	16.418	3.1	1.2	1.3	94.4	100

285 (B2U)--V	16.51	0	1.8	0	98.2	100
286 A1U)--V	16.585	0	0	0	100	100
287 (B1G)--V	16.604	0.1	14.4	7.5	78	100
288 (B1U)--V	17.27	0	0	2.3	97.7	100
289 (EG)--V	17.385	0	0.6	0.3	99.1	100
290 (EG)--V	17.385	0	0.6	0.3	99.1	100
291 A2U)--V	17.568	0.7	0.4	4.2	94.7	100
292 (A1G)--V	17.683	6.1	23	3.8	67.1	100
293 (B2U)--V	18.842	0	1.1	0	98.9	100
294 (EG)--V	18.881	0	1.8	2	96.2	100
295 (EG)--V	18.881	0	1.8	2	96.2	100
296 A1U)--V	19.1	0	0	0	100	100
297 (EU)--V	19.204	5.7	15.5	7.1	71.6	100
298 (EU)--V	19.204	5.7	15.5	7.1	71.6	100
299 (B1U)--V	19.621	0	0	3.5	96.5	100
300 (EG)--V	20.022	0.3	36.4	6.5	56.7	100
301 (EG)--V	20.022	0.3	36.4	6.5	56.7	100
302 (B2G)--V	20.196	0	0.1	3.4	96.5	100
303 (EU)--V	20.443	0.1	1	1.6	97.3	100
304 (EU)--V	20.443	0.1	1	1.6	97.3	100
305 (A1G)--V	20.597	0.1	0.3	0.9	98.7	100
306 A2U)--V	20.787	1.2	12.3	55.1	31.4	100
307 (B2G)--V	20.903	0	2.3	1.8	95.9	100
308 (A2G)--V	21.141	0	0.3	0.8	98.9	100
309 (EG)--V	21.201	0	1.7	0.4	97.9	100
310 (EG)--V	21.201	0	1.7	0.4	97.9	100
311 (EU)--V	21.225	0.1	0.1	1.1	98.7	100
312 (EU)--V	21.225	0.1	0.1	1.1	98.7	100
313 (A2G)--V	21.578	0	1.5	1.2	97.3	100
314 (EU)--V	21.67	0	0.8	0.4	98.7	100
315 (EU)--V	21.67	0	0.8	0.4	98.7	100
316 B1G)--V	21.708	0	0.9	0.4	98.7	100
317 (B2G)--V	21.832	0	9.4	8.4	82.1	100
318 (B2G)--V	22.219	0	1.5	4.6	93.9	100
319 (A1G)--V	22.257	0.4	9	7.3	83.3	100
320 (EU)--V	22.343	0.2	1.8	3.5	94.5	100
321 (EU)--V	22.343	0.2	1.8	3.5	94.5	100
322 (B2U)--V	22.534	0	67.8	0	32.2	100
323 (A2G)--V	22.625	0	0.7	9.5	89.7	100
324 (A1U)--V	22.78	0	0	0	100	100
325 (EU)--V	22.918	0.1	0.7	3.2	95.9	100
326 (EU)--V	22.918	0.1	0.7	3.2	95.9	100
327 (B1G)--V	22.924	0	0.5	0	99.5	100
328 (A1G)--V	23.04	2.6	2.8	27.4	67.1	100
329 (EG)--V	23.349	0.1	14.2	41.3	44.4	100
330 (EG)--V	23.349	0.1	14.2	41.3	44.4	100
331 B1U)--V	23.408	0	0	63.2	36.8	100
332 (B1G)--V	23.595	0	20.3	10.4	69.3	100

333 (EU)--V	23.736	0.4	3.6	7.9	88.1	100
334 (EU)--V	23.736	0.4	3.6	7.9	88.1	100
335 (A1G)--V	23.765	0.8	9.8	6	83.4	100
336 (EU)--V	24.221	0.3	9	4.9	85.8	100
337 (EU)--V	24.221	0.3	9	4.9	85.8	100
338 (A2G)--V	24.345	0	0	0	100	100
339 (B1G)--V	24.495	0	0.3	0.3	99.4	100
340 (EU)--V	24.852	0.3	0.1	3.7	95.9	100
341 (EU)--V	24.852	0.3	0.1	3.7	95.9	100
342 (B2G)--V	25.374	0	0	0.6	99.4	100
343 (A2U)--V	25.393	4.5	42.7	16	36.8	100
344 (A2G)--V	25.454	0	0	1.7	98.3	100
345 (EU)--V	25.569	0	0.8	2.4	96.8	100
346 (EU)--V	25.569	0	0.8	2.4	96.8	100
347 (B2G)--V	25.957	0	1.2	2.3	96.6	100
348 (B1G)--V	26.151	0	8.3	1.7	90	100
349 (EU)--V	26.336	0.5	7.1	3.8	88.6	100
350 (EU)--V	26.336	0.5	7.1	3.8	88.6	100
351 A1G)--V	26.736	0	3.4	3.5	93.1	100
352 (EU)--V	26.744	0	6.3	5.8	87.9	100
353 (EU)--V	26.744	0	6.3	5.8	87.9	100
354 (A1G)--V	27.045	0.2	5.9	6.2	87.6	100
355 (B2G)--V	27.527	0	7	3.9	89.1	100
356 (EU)--V	27.941	0	2.1	2.8	95.2	100
357 (EU)--V	27.941	0	2.1	2.8	95.2	100
358 (A2G)--V	28.062	0	0.8	0.2	99.1	100
359 (A2G)--V	28.949	0	2.6	2	95.4	100
360 (B1G)--V	29.057	0	1.1	15.1	83.8	100
361 (EU)--V	29.205	0.1	1.2	0.7	98.1	100
362 (EU)--V	29.205	0.1	1.2	0.7	98.1	100
363 (B2G)--V	29.309	0	0.8	4.5	94.7	100
364 (B1G)--V	29.592	0	5.2	12.3	82.5	100
365 (A1G)--V	29.866	0.9	6.5	3.7	88.9	100
366 (EU)--V	30.014	0.2	5.6	2.9	91.3	100
367 (EU)--V	30.014	0.2	5.6	2.9	91.3	100
368 (B2G)--V	30.342	0	1.3	2.8	95.9	100
369 (A1G)--V	31.061	5.4	3.7	0.3	90.6	100
370 (B2U)--V	31.145	0	8	8.4	83.6	100
371 (EU)--V	31.247	1	6.7	4.6	87.6	100
372 (EU)--V	31.247	1	6.7	4.6	87.6	100
373 (A2G)--V	31.45	0	1.6	13.9	84.5	100
374 (EG)--V	31.532	0.2	5.4	14.4	80	100
375 (EG)--V	31.532	0.2	5.4	14.4	80	100
376 B1G)--V	31.983	0.3	10.3	9.2	80.1	100
377 (A2U)--V	32.15	0.2	0.8	10.7	88.2	100
378 (EU)--V	32.463	0.2	3.5	9	87.2	100
379 (EU)--V	32.463	0.2	3.5	9	87.2	100
380 (B2G)--V	32.691	0	1.7	2	96.4	100

381 A1U)--V	33.031	0	19.9	18.3	61.8	100
382 (EG)--V	33.064	0	8.6	10	81.4	100
383 (EG)--V	33.064	0	8.6	10	81.4	100
384 (B2U)--V	33.148	0	6.3	9.9	83.8	100
385 (EU)--V	33.483	0.2	1.8	13	85.1	100
386 (EU)--V	33.483	0.2	1.8	13	85.1	100
387 (A2G)--V	33.942	0	0.7	8.2	91.1	100
388 (B1U)--V	34.054	0	5.2	6.6	88.3	100
389 (EG)--V	34.139	0.2	5.3	7	87.5	100
390 (EG)--V	34.139	0.2	5.3	7	87.5	100
391 B1G)--V	34.243	0	0.4	4.4	95.2	100
392 (A1U)--V	34.366	0	3.7	5.6	90.7	100
393 (A2U)--V	34.898	4.2	26.9	17.6	51.3	100
394 (A1G)--V	34.973	3.4	5.5	0.1	91	100
395 (EG)--V	35.013	2.1	18.6	7.9	71.4	100
396 (EG)--V	35.013	2.1	18.6	7.9	71.4	100
397 (EU)--V	35.114	0.1	4	0.6	95.3	100
398 (EU)--V	35.114	0.1	4	0.6	95.3	100
399 (B1G)--V	35.168	0	6	0.2	93.8	100
400 (EU)--V	36.004	0.3	6.8	0.2	92.8	100
401 (EU)--V	36.004	0.3	6.8	0.2	92.8	100
402 (B2U)--V	36.642	0	28.4	0.7	70.9	100
403 (A1G)--V	37.035	0.1	0.4	0	99.5	100
404 (EU)--V	37.281	0.1	1.2	1.5	97.3	100
405 (EU)--V	37.281	0.1	1.2	1.5	97.3	100
406 A2G)--V	37.288	0	3.1	17.3	79.6	100
407 (B2G)--V	37.304	0	0.1	0.4	99.5	100
408 (B1G)--V	37.348	0	0.1	1.1	98.8	100
409 (EG)--V	37.393	0.2	4.1	6.1	89.6	100
410 (EG)--V	37.393	0.2	4.1	6.1	89.6	100
411 A2U)--V	37.412	0.6	2.1	1.9	95.5	100
412 (B2U)--V	37.484	0	0.2	0.7	99.1	100
413 (EG)--V	37.737	0.5	12.4	12.1	75.1	100
414 (EG)--V	37.737	0.5	12.4	12.1	75.1	100
415 (A2U)--V	37.963	2.3	10	0.7	87	100
416 B2U)--V	38.302	0	2.2	0.7	97.1	100
417 (B1U)--V	38.31	0	18.4	24.1	57.5	100
418 (EG)--V	38.571	0.3	6.7	3.5	89.5	100
419 (EG)--V	38.571	0.3	6.7	3.5	89.5	100
420 (A1U)--V	38.612	0	0	0	100	100
421 B1U)--V	38.671	0	3.9	5.6	90.4	100
422 (EG)--V	38.689	0.5	12.9	8	78.5	100
423 (EG)--V	38.689	0.5	12.9	8	78.5	100
424 (EU)--V	38.916	0	1.3	0.7	98	100
425 (EU)--V	38.916	0	1.3	0.7	98	100
426 A2G)--V	39.53	0	4.3	0	95.6	100
427 (A2U)--V	39.53	8	39.3	6	46.7	100
428 (A2G)--V	40.523	0	2	4.2	93.8	100

429 (B2G)--V	41.211	0	0.1	1.5	98.4	100
430 (EU)--V	41.278	0.2	4	0.1	95.7	100
431 (EU)--V	41.278	0.2	4	0.1	95.7	100
432 (A1G)--V	41.554	0.1	40.4	0.7	58.8	100
433 (EU)--V	41.865	0.8	13.9	2.7	82.6	100
434 (EU)--V	41.865	0.8	13.9	2.7	82.6	100
435 (A1G)--V	42.775	0.4	42.7	1.2	55.7	100
436 B1G)--V	43.261	0	32.4	2.6	65	100
437 (B2G)--V	44.354	0	0.2	19.1	80.7	100
438 (EU)--V	44.855	0.8	1	43.2	55	100
439 (EU)--V	44.855	0.8	1	43.2	55	100
440 (A1G)--V	45.126	1	0.7	53	45.3	100
441 B1G)--V	45.621	0	43.8	10.6	45.6	100
442 (EU)--V	45.944	0.2	36.1	4.3	59.4	100
443 (EU)--V	45.944	0.2	36.1	4.3	59.4	100
444 (B1U)--V	45.994	0	1.5	12.4	86.2	100
445 (A1G)--V	46.114	0.6	44.9	3.6	50.9	100
446 (EG)--V	46.308	0	2.5	9.9	87.6	100
447 (EG)--V	46.308	0	2.5	9.9	87.6	100
448 (A1U)--V	46.768	0	3.6	2.7	93.8	100
449 (B1G)--V	47.194	0	53.6	1.4	45	100
450 (EU)--V	47.667	0.1	21.9	2.3	75.6	100
451 (EU)--V	47.667	0.1	21.9	2.3	75.6	100
452 (B2G)--V	47.679	0	0.1	10.9	88.9	100
453 (A1G)--V	47.777	0.1	20.6	3.9	75.4	100
454 (EU)--V	48.008	0.1	0.8	23.6	75.5	100
455 (EU)--V	48.008	0.1	0.8	23.6	75.5	100
456 A2U)--V	48.136	0.5	10.6	25	63.9	100
457 (A2G)--V	48.174	0	0.5	0	99.5	100
458 (A1G)--V	48.53	0.6	19	40.4	40	100
459 (EU)--V	48.994	0.1	10.5	1.5	88	100
460 (EU)--V	48.994	0.1	10.5	1.5	88	100
461 B1G)--V	49.012	0	31.3	5.1	63.6	100
462 (EG)--V	49.19	0.4	16	17.5	66.1	100
463 (EG)--V	49.19	0.4	16	17.5	66.1	100
464 (A2G)--V	49.457	0	0	0.1	99.9	100
465 (B2G)--V	49.939	0	0	0.9	99.1	100
466 A1G)--V	49.976	0	10.9	39	50.1	100
467 (EU)--V	50.008	0	0.4	0.9	98.6	100
468 (EU)--V	50.008	0	0.4	0.9	98.6	100
469 (B2U)--V	50.224	0	26.4	11.6	62.1	100
470 (EU)--V	50.291	1.9	5.8	20.6	71.7	100
471 (EU)--V	50.291	1.9	5.8	20.6	71.7	100
472 (B1G)--V	50.464	0	15.9	5.6	78.5	100
473 (B1G)--V	50.485	0	10.8	4	85.2	100
474 (EU)--V	50.805	3	13	9.1	74.9	100
475 (EU)--V	50.805	3	13	9.1	74.9	100
476 (EU)--V	51.405	13.9	31.5	0.5	54	100

477 (EU)--V	51.405	13.9	31.5	0.5	54	100
478 (A1G)--V	51.739	0.5	7.3	12.8	79.4	100
479 (A2G)--V	51.866	0	0	0.6	99.3	100
480 (B2G)--V	52.211	0	0.3	8.2	91.4	100
481 B2U)--V	52.465	0	26.7	14.2	59.1	100
482 (EU)--V	52.629	0	3.4	1.3	95.3	100
483 (EU)--V	52.629	0	3.4	1.3	95.3	100
484 (A1G)--V	53.368	0	18.2	14.2	67.6	100
485 (EU)--V	53.373	0.1	6.1	3.6	90.1	100
486 (EU)--V	53.373	0.1	6.1	3.6	90.1	100
487 (EG)--V	53.666	1.2	28.4	17.2	53.3	100
488 (EG)--V	53.666	1.2	28.4	17.2	53.3	100
489 (B1G)--V	53.797	0	28.5	4	67.5	100
490 (B1U)--V	54.813	0	2.5	29.1	68.5	100
491 A1U)--V	54.854	0	24.9	11.3	63.9	100
492 (A2G)--V	54.855	0	8.6	4.7	86.6	100
493 (EG)--V	54.88	3.8	4.8	20.3	71.1	100
494 (EG)--V	54.88	3.8	4.8	20.3	71.1	100
495 (A2U)--V	54.92	0.4	4.9	20.7	74	100
496 B2G)--V	55.057	0	0.2	0.2	99.6	100
497 (EU)--V	55.324	0.1	0.8	1.5	97.5	100
498 (EU)--V	55.324	0.1	0.8	1.5	97.5	100
499 (A2G)--V	55.557	0	2.6	2.6	94.8	100
500 (EU)--V	55.701	0	2.3	4.3	93.3	100
501 (EU)--V	55.701	0	2.3	4.3	93.3	100
502 (B1G)--V	56.214	0	4.9	9.3	85.7	100
503 (B2G)--V	56.371	0	0.3	6	93.7	100
504 (EU)--V	56.595	0.1	0.7	3.3	95.9	100
505 (EU)--V	56.595	0.1	0.7	3.3	95.9	100
506 A1G)--V	56.847	0.7	4.3	0.8	94.1	100
507 (EG)--V	56.89	45.7	14.5	0.8	38.9	100
508 (EG)--V	56.89	45.7	14.5	0.8	38.9	100
509 (B1U)--V	57.454	0	9.9	13.3	76.8	100
510 (EG)--V	57.565	30.8	8.9	4.8	55.6	100
511 (EG)--V	57.565	30.8	8.9	4.8	55.6	100
512 (A1U)--V	58.326	0	5.4	4.9	89.8	100
513 (B2U)--V	58.444	0	1.1	0	98.9	100
514 (A2G)--V	58.554	0	0.1	0.3	99.6	100
515 (EU)--V	58.74	0	3.9	6.8	89.2	100
516 (EU)--V	58.74	0	3.9	6.8	89.2	100
517 (EG)--V	58.994	0.2	8.8	0.1	90.9	100
518 (EG)--V	58.994	0.2	8.8	0.1	90.9	100
519 (B1U)--V	59.108	0	6.4	1.5	92.1	100
520 (EG)--V	59.277	1.7	1.5	6.3	90.5	100
521 (EG)--V	59.277	1.7	1.5	6.3	90.5	100
522 (A2U)--V	59.372	0.3	30.6	6	63.1	100
523 (A2U)--V	59.459	0.1	12.9	0.8	86.3	100
524 (A1U)--V	59.586	0	0.2	4.8	95	100



525 (B2G)--V	59.674	0	0.2	11.9	87.9	100
526 A2G)--V	59.679	0	3.2	1.3	95.5	100
527 (EU)--V	60.161	2.1	13.3	16	68.5	100
528 (EU)--V	60.161	2.1	13.3	16	68.5	100
529 (B1G)--V	60.415	0	36.1	16.6	47.3	100
530 (B2U)--V	60.483	0	2.5	1.2	96.4	100
531 (EG)--V	60.498	0	8.6	4.5	86.9	100
532 (EG)--V	60.498	0	8.6	4.5	86.9	100
533 (A1G)--V	61.416	0.1	1.2	17.6	81.1	100
534 (B2G)--V	61.782	5.5	5.4	4.1	85	100
535 (B1U)--V	62.293	0	18.1	1.7	80.2	100
536 (EU)--V	62.836	0.1	1.9	25.9	72.1	100
537 (EU)--V	62.836	0.1	1.9	25.9	72.1	100
538 (EG)--V	63.34	0.6	15.4	8.7	75.3	100
539 (EG)--V	63.34	0.6	15.4	8.7	75.3	100
540 (A2G)--V	63.483	0	0.1	0	99.9	100
541 (EU)--V	63.862	0	0.2	0.6	99.2	100
542 (EU)--V	63.862	0	0.2	0.6	99.2	100
543 (B2G)--V	64.148	0	2.5	25.2	72.3	100
544 (B1G)--V	64.162	0	1.7	0.1	98.2	100
545 (B2G)--V	64.647	0.4	3.4	3.1	93.1	100
546 A1U)--V	65.528	0	2.6	6.7	90.7	100
547 (A1G)--V	65.632	2.1	16.7	1.6	79.6	100
548 (A2U)--V	65.675	0.2	8.7	19.1	72	100
549 (EU)--V	65.929	0.2	8.8	11.1	79.9	100
550 (EU)--V	65.929	0.2	8.8	11.1	79.9	100
551 (EG)--V	66.741	0	7.5	10	82.5	100
552 (EG)--V	66.741	0	7.5	10	82.5	100
553 (A1U)--V	67.815	0	13.5	12.4	74.1	100
554 (B1U)--V	67.941	0	12.2	8.3	79.5	100
555 (B1G)--V	69.045	0.7	56.4	4.9	38	100
556 A1G)--V	69.16	2.7	18.1	35.8	43.4	100
557 (A2G)--V	69.469	0	0.7	0.3	99	100
558 (EG)--V	69.724	0.3	7.2	10.8	81.7	100
559 (EG)--V	69.724	0.3	7.2	10.8	81.7	100
560 (EU)--V	69.842	0	0.2	0.5	99.3	100
561 (EU)--V	69.842	0	0.2	0.5	99.3	100
562 (B2G)--V	69.85	0	0.3	0.1	99.6	100
563 (EU)--V	70.096	0.1	17.6	11.8	70.5	100
564 (EU)--V	70.096	0.1	17.6	11.8	70.5	100
565 (B1G)--V	70.32	0	0.4	3.6	96.1	100
566 (EU)--V	70.477	0.1	25.4	26.9	47.5	100
567 (EU)--V	70.477	0.1	25.4	26.9	47.5	100
568 (A1G)--V	70.56	2.4	11.6	24	62	100
569 (B1U)--V	70.568	0	0.2	4.2	95.7	100
570 (A2G)--V	70.635	0	2.1	1.7	96.2	100
571 (EU)--V	70.82	0	10.4	8.5	81	100
572 (EU)--V	70.82	0	10.4	8.5	81	100

573(B1G)--V	70.956	0	28.1	3.5	68.4	100
574(A1G)--V	71.41	6.2	6.7	0.5	86.6	100
575(B2U)--V	71.673	0	15.9	30.7	53.3	100
576 A1U)--V	71.827	0	5.5	16.7	77.8	100
577(EG)--V	71.875	0.2	9.9	22.1	67.8	100
578(EG)--V	71.875	0.2	9.9	22.1	67.8	100
579(B1G)--V	72.002	0.2	27.3	4	68.4	100
580(EU)--V	72.049	0.1	41.2	14.3	44.5	100
581(EU)--V	72.049	0.1	41.2	14.3	44.5	100
582(A1G)--V	72.273	0.1	53.9	20.2	25.7	100
583(B2G)--V	73.042	0	0.2	7.2	92.6	100
584(B2G)--V	73.401	0.1	3.9	20.9	75.1	100
585(EU)--V	73.781	0	2.1	6.6	91.3	100
586(EU)--V	73.781	0	2.1	6.6	91.3	100
587(A2G)--V	74.136	0	0.9	6.5	92.6	100
588(B1G)--V	74.188	1.2	52	4.5	42.3	100
589(B2G)--V	74.618	0	0.1	0.3	99.6	100
590(EU)--V	75.351	0	2.6	4.7	92.6	100
591(EU)--V	75.351	0	2.6	4.7	92.6	100
592(EU)--V	76.9	0.1	7.4	4.7	87.7	100
593(EU)--V	76.9	0.1	7.4	4.7	87.7	100
594(A2G)--V	77.075	0	1.2	2.6	96.2	100
595(A1G)--V	77.331	0.3	21.2	25.3	53.2	100
596(EU)--V	77.411	0.4	6.1	5.3	88.2	100
597(EU)--V	77.411	0.4	6.1	5.3	88.2	100
598(B2G)--V	78.959	0	0.1	7.8	92	100
599(B1G)--V	78.997	0.8	6.7	6	86.5	100
600(A2G)--V	79.965	0	0.3	0	99.6	100
601 A1G)--V	80.368	0.5	3.9	4.7	90.9	100
602(EU)--V	80.548	0.1	9.8	10.7	79.4	100
603(EU)--V	80.548	0.1	9.8	10.7	79.4	100
604(A2G)--V	81.252	0	15.4	4.6	80.1	100
605(B2G)--V	82.405	0	2.3	2.5	95.2	100
606(EU)--V	82.872	0	1	5.2	93.8	100
607(EU)--V	82.872	0	1	5.2	93.8	100
608(EU)--V	85.256	0.2	7.4	19.7	72.7	100
609(EU)--V	85.256	0.2	7.4	19.7	72.7	100
610(B1G)--V	86.577	0.8	5.2	25.8	68.2	100
611 A1G)--V	88.463	0.4	4.1	55.2	40.3	100
612(B2G)--V	88.951	0	1	1.8	97.2	100
613(EU)--V	90.129	0	1.5	3	95.6	100
614(EU)--V	90.129	0	1.5	3	95.6	100
615(A2G)--V	90.846	0	6.6	11.8	81.6	100
616 A2G)--V	90.956	0	2.5	2.4	95.1	100
617(EU)--V	92.866	0	5.5	4.4	90.1	100
618(EU)--V	92.866	0	5.5	4.4	90.1	100
619(B2G)--V	93.542	0	4	3	93	100

## BPW91 Exchange Correlation Functional

Orbital	Index	E, eV	Zn	NZn	Nmeso	Pc	Total
	1 A1G)--O	-9408.93	100	0	0	0	100
	2 (A1G)--O	-1133.97	100	0	0	0	100
	3 (A2U)--O	-1000.19	100	0	0	0	100
	4 (EU)--O	-1000	100	0	0	0	100
	5 (EU)--O	-1000	100	0	0	0	100
	6 (EU)--O	-381.842	0	99.8	0	0.2	100
	7 (EU)--O	-381.842	0	99.8	0	0.2	100
	8 (B1G)--O	-381.842	0	99.8	0	0.2	100
	9 (A1G)--O	-381.842	0	99.9	0	0.1	100
	10 (B2G)--O	-381.514	0	0	99.7	0.3	100
	11 (EU)--O	-381.514	0	0	99.7	0.2	100
	12 (EU)--O	-381.514	0	0	99.7	0.2	100
	13 (A1G)--O	-381.514	0	0	99.8	0.2	100
	14 (B2G)--O	-271.639	0	0	0.2	99.8	100
	15 (EU)--O	-271.639	0	0	0.1	99.9	100
	16 (EU)--O	-271.639	0	0	0.1	99.9	100
	17 (A1G)--O	-271.638	0	0	0	100	100
	18 (A2G)--O	-271.638	0	0	0	100	100
	19 (EU)--O	-271.637	0	0	0	100	100
	20 (EU)--O	-271.637	0	0	0	100	100
	21 B1G)--O	-271.637	0	0	0	100	100
	22 (EU)--O	-269.887	0	0	0	100	100
	23 (EU)--O	-269.887	0	0	0	100	100
	24 (A1G)--O	-269.887	0	0	0	100	100
	25 (B1G)--O	-269.887	0	0	0	100	100
	26 A2G)--O	-269.882	0	0	0	100	100
	27 (EU)--O	-269.882	0	0	0	100	100
	28 (EU)--O	-269.882	0	0	0	100	100
	29 (B2G)--O	-269.882	0	0	0	100	100
	30 (B1G)--O	-269.87	0	0	0	100	100
	31 (EU)--O	-269.87	0	0	0	100	100
	32 (EU)--O	-269.87	0	0	0	100	100
	33 (A1G)--O	-269.87	0	0	0	100	100
	34 (A2G)--O	-269.869	0	0	0	100	100
	35 (EU)--O	-269.869	0	0	0	100	100
	36 (EU)--O	-269.869	0	0	0	100	100
	37 (B2G)--O	-269.869	0	0	0	100	100
	38 (B1G)--O	-269.86	0	0	0	100	100
	39 (EU)--O	-269.86	0	0	0	100	100
	40 (EU)--O	-269.86	0	0	0	100	100
	41 A1G)--O	-269.86	0	0	0	100	100
	42 (A2G)--O	-269.854	0	0	0	100	100
	43 (EU)--O	-269.854	0	0	0	100	100
	44 (EU)--O	-269.854	0	0	0	100	100

45 (B2G)--O	-269.854	0	0	0	100	100
46 A1G)--O	-124.952	100	0	0	0	100
47 (A2U)--O	-82.55	100	0	0	0	100
48 (EU)--O	-82.228	100	0	0	0	100
49 (EU)--O	-82.228	100	0	0	0	100
50 (A1G)--O	-25.107	0.4	40	25.2	34.4	100
51 (EU)--O	-24.74	0.2	39.2	24.8	35.8	100
52 (EU)--O	-24.74	0.2	39.2	24.8	35.8	100
53 (B1G)--O	-24.028	0.1	59.5	0.7	39.6	100
54 (B2G)--O	-23.454	0	1.8	70.1	28.1	100
55 (EU)--O	-22.407	0	17.8	50.6	31.6	100
56 (EU)--O	-22.407	0	17.8	50.6	31.6	100
57 (A1G)--O	-21.602	0.1	17	50.2	32.6	100
58 (A1G)--O	-21.15	0.4	21.7	8.1	69.8	100
59 (EU)--O	-21.133	0.1	14.6	1.2	84.2	100
60 (EU)--O	-21.133	0.1	14.6	1.2	84.2	100
61 B1G)--O	-21.119	0.1	13.1	0	86.8	100
62 (A2G)--O	-19.089	0	2.8	6.8	90.4	100
63 (A1G)--O	-18.77	0.7	12.8	0.3	86.3	100
64 (EU)--O	-18.74	0.1	14	4.2	81.8	100
65 (EU)--O	-18.74	0.1	14	4.2	81.8	100
66 (EU)--O	-18.629	0	4.5	1.3	94.2	100
67 (EU)--O	-18.629	0	4.5	1.3	94.2	100
68 (B1G)--O	-18.617	0.4	19.4	0.7	79.6	100
69 (B2G)--O	-18.551	0	0	1.8	98.2	100
70 (A2G)--O	-17.735	0	5.5	8.5	86	100
71 (EU)--O	-17.078	0	7	18.4	74.5	100
72 (EU)--O	-17.078	0	7	18.4	74.5	100
73 (B1G)--O	-15.725	0.7	11.5	20.2	67.6	100
74 (A1G)--O	-15.612	2	11.7	0.4	85.9	100
75 (EU)--O	-15.447	0.2	11.2	0.4	88.2	100
76 (EU)--O	-15.447	0.2	11.2	0.4	88.2	100
77 (B2G)--O	-15.284	0	3.1	13.7	83.2	100
78 (B1G)--O	-15.202	0.6	5.5	9.7	84.2	100
79 (EU)--O	-14.569	0	6.1	3.2	90.7	100
80 (EU)--O	-14.569	0	6.1	3.2	90.7	100
81 B2G)--O	-14.499	1.5	31.2	22.9	44.4	100
82 (A2G)--O	-14.328	0	6	1.5	92.5	100
83 (A1G)--O	-13.576	3.1	8	1.4	87.5	100
84 (EU)--O	-13.423	0	18.5	13.7	67.9	100
85 (EU)--O	-13.423	0	18.5	13.7	67.9	100
86 (EU)--O	-13.024	0.4	13.7	18.4	67.5	100
87 (EU)--O	-13.024	0.4	13.7	18.4	67.5	100
88 (B1G)--O	-12.983	5.4	12.4	5.5	76.7	100
89 (A2G)--O	-12.225	0	24.6	14.8	60.6	100
90 (B2G)--O	-12.149	0.9	2.1	1.6	95.4	100
91 A1G)--O	-11.781	19.3	21.1	1.3	58.3	100
92 (EU)--O	-11.668	0	2.5	4	93.4	100
93 (EU)--O	-11.668	0	2.5	4	93.4	100
94 (B1G)--O	-11.57	31	19.2	0.2	49.6	100
95 (A2U)--O	-11.282	0.4	25.3	17.9	56.4	100

96 (EU)--O	-11.247	0.6	13.6	1.1	84.6	100
97 (EU)--O	-11.247	0.6	13.6	1.1	84.6	100
98 (A2G)--O	-11.168	0	0.5	7.1	92.3	100
99 (EG)--O	-10.996	18	24.9	12.2	44.8	100
100 (EG)--O	-10.996	18	24.9	12.2	44.8	100
101 A1G)--O	-10.73	7.3	8	5.5	79.2	100
102 (B1G)--O	-10.663	23.7	10.7	1.7	63.8	100
103 (EU)--O	-10.594	0	1.1	1.4	97.4	100
104 (EU)--O	-10.594	0	1.1	1.4	97.4	100
105 (B2G)--O	-10.59	0.3	0.1	0.7	98.9	100
106 A1G)--O	-10.341	43.7	5.9	2.2	48.2	100
107 (A2G)--O	-10.32	0	0.6	4	95.4	100
108 (EU)--O	-10.224	0.3	5.3	4.4	90	100
109 (EU)--O	-10.224	0.3	5.3	4.4	90	100
110 (B2U)--O	-10.172	0	26.5	0	73.5	100
111 (EG)--O	-9.928	88.3	1.2	1.9	8.6	100
112 (EG)--O	-9.928	88.3	1.2	1.9	8.6	100
113 (B2G)--O	-9.827	49.4	6.2	0.8	43.5	100
114 (B1G)--O	-9.826	17.7	1.4	3.1	77.8	100
115 (B1U)--O	-9.309	0	0.1	50.6	49.3	100
116 A1G)--O	-9.298	63.6	11.8	2.4	22.2	100
117 (B2G)--O	-8.82	1.5	0.2	1.6	96.7	100
118 (EG)--O	-8.789	2.4	1.9	15.2	80.5	100
119 (EG)--O	-8.789	2.4	1.9	15.2	80.5	100
120 (A2U)--O	-8.768	0.3	7.1	4	88.6	100
121 (EU)--O	-8.749	0	1.6	1.9	96.5	100
122 (EU)--O	-8.749	0	1.6	1.9	96.5	100
123 (A2G)--O	-8.555	0	1.9	1.1	97	100
124 (EU)--O	-8.405	4.5	33.2	2.5	59.7	100
125 (EU)--O	-8.405	4.5	33.2	2.5	59.7	100
126 A1G)--O	-8.397	0	1.7	3	95.3	100
127 (B2U)--O	-8.387	0	25.6	0	74.4	100
128 (B1G)--O	-8.043	1.7	0.6	3	94.8	100
129 (EU)--O	-8.04	2.6	16.9	6.4	74.1	100
130 (EU)--O	-8.04	2.6	16.9	6.4	74.1	100
131 (EG)--O	-7.719	3.3	19.5	20	57.2	100
132 (EG)--O	-7.719	3.3	19.5	20	57.2	100
133 (A1G)--O	-6.942	0.2	18.8	54.1	26.9	100
134 (A1U)--O	-6.731	0	0	0	99.9	100
135 (A2U)--O	-6.289	3	48	23.7	25.3	100
136 (EU)--O	-6.26	0.2	18	50.6	31.2	100
137 (EU)--O	-6.26	0.2	18	50.6	31.2	100
138 (B1U)--O	-6.237	0	0	5.3	94.7	100
139 (EG)--O	-6.216	0	0.4	10	89.5	100
140 (EG)--O	-6.216	0	0.4	10	89.5	100
141 A2U)--O	-6.122	0.1	4.1	37	58.9	100
142 (EG)--O	-6.003	2.1	28.6	1.6	67.7	100
143 (EG)--O	-6.003	2.1	28.6	1.6	67.7	100
144 (B2U)--O	-5.992	0	25.9	0	74.1	100
145 (B2G)--O	-5.783	0.7	12.2	61.8	25.3	100
146 B1G)--O	-5.319	24.8	48.4	0.8	26.1	100

147 (A1U)--O	-4.659	0	0.1	0.1	99.8	100
148 (EG)--V	-3.203	0.4	13.3	19.8	66.5	100
149 (EG)--V	-3.203	0.4	13.3	19.8	66.5	100
150 (B1U)--V	-1.783	0	0	25.1	74.8	100
151 B2U)--V	-1.562	0	19.6	0	80.3	100
152 (A2U)--V	-1.417	5.2	1.3	5.4	88.1	100
153 (EG)--V	-1.291	0.1	5.6	3.7	90.6	100
154 (EG)--V	-1.291	0.1	5.6	3.7	90.6	100
155 (A1U)--V	-0.115	0	0	0	100	100
156 (EG)--V	-0.056	0	1.8	0.9	97.3	100
157 (EG)--V	-0.056	0	1.8	0.9	97.3	100
158 (A2U)--V	0.349	60.2	6.1	3.5	30.2	100
159 (B2U)--V	0.502	0	19.4	0.1	80.5	100
160 (A1G)--V	0.601	67.7	19.5	0.5	12.2	100
161 B1U)--V	0.703	0	0.1	18.5	81.4	100
162 (EG)--V	1.989	0.1	14.4	15.9	69.5	100
163 (EG)--V	1.989	0.1	14.4	15.9	69.5	100
164 (A1G)--V	2.066	0.3	0.1	1.9	97.7	100
165 (EU)--V	2.133	4.5	0.9	1	93.6	100
166 (EU)--V	2.133	4.5	0.9	1	93.6	100
167 (B1G)--V	2.254	0	0	0.1	99.9	100
168 (EU)--V	2.534	63.9	9.9	2.6	23.5	100
169 (EU)--V	2.534	63.9	9.9	2.6	23.5	100
170 (A2U)--V	2.756	26.5	18.2	16.5	38.8	100
171 B2G)--V	3.096	0	1.1	0.2	98.7	100
172 (EU)--V	3.283	0.1	1.2	0.1	98.5	100
173 (EU)--V	3.283	0.1	1.2	0.1	98.5	100
174 (A1G)--V	3.352	33.2	0.4	10.6	55.9	100
175 (A2G)--V	3.51	0	0.7	0	99.2	100
176 A1U)--V	3.631	0	0	0	100	100
177 (EG)--V	3.809	0	0.9	4.1	95	100
178 (EG)--V	3.809	0	0.9	4.1	95	100
179 (B1U)--V	3.83	0	0	4.6	95.4	100
180 (EU)--V	3.97	1.6	0.1	3.3	94.9	100
181 (EU)--V	3.97	1.6	0.1	3.3	94.9	100
182 (B2G)--V	3.986	0	0.1	5.2	94.7	100
183 (A1G)--V	4.267	33.9	0.9	0.3	64.9	100
184 (B1G)--V	4.314	0	6.5	0.4	93.1	100
185 (EU)--V	4.316	1.5	2.3	0.2	95.9	100
186 (EU)--V	4.316	1.5	2.3	0.2	95.9	100
187 (A2G)--V	4.515	0	0.1	0	99.8	100
188 (EU)--V	4.972	6.3	8.7	3.5	81.6	100
189 (EU)--V	4.972	6.3	8.7	3.5	81.6	100
190 (B2G)--V	4.993	0.1	3.3	9.1	87.5	100
191 B1G)--V	5.129	0	25.6	3.7	70.7	100
192 (A1G)--V	5.164	0.1	0.6	1	98.3	100
193 (EU)--V	5.665	0.3	0.6	2.2	96.8	100
194 (EU)--V	5.665	0.3	0.6	2.2	96.8	100
195 (A2U)--V	5.739	89.8	2.5	0.9	6.8	100
196 A2G)--V	5.828	0	5.9	0.6	93.5	100
197 (EU)--V	6.052	1	0.3	5.8	92.8	100

198 (EU)--V	6.052	1	0.3	5.8	92.8	100
199 (B2G)--V	6.054	0	0.3	12.2	87.5	100
200 (B1G)--V	6.36	0	2.6	0	97.4	100
201 A2G)--V	6.404	0	0.3	0	99.7	100
202 (A1G)--V	6.642	9.6	10.9	20.4	59	100
203 (EU)--V	6.733	1.7	6.2	2.3	89.8	100
204 (EU)--V	6.733	1.7	6.2	2.3	89.8	100
205 (EU)--V	7.062	1	5.7	2.6	90.8	100
206 (EU)--V	7.062	1	5.7	2.6	90.8	100
207 (A1G)--V	7.216	5.5	0.6	2.5	91.4	100
208 (B2G)--V	7.736	0	0.7	4.1	95.2	100
209 (B1G)--V	7.819	0	0.3	0	99.6	100
210 (EU)--V	8.12	0.5	1.8	12	85.7	100
211 (EU)--V	8.12	0.5	1.8	12	85.7	100
212 (A1G)--V	8.362	0.3	1.3	2	96.5	100
213 (EU)--V	8.383	1.7	4.8	2.4	91.1	100
214 (EU)--V	8.383	1.7	4.8	2.4	91.1	100
215 (B2G)--V	8.722	0	5.6	23.4	71	100
216 B1G)--V	8.916	0	3.4	0.1	96.4	100
217 (B2G)--V	9.201	0	0.4	15.8	83.8	100
218 (A2G)--V	9.412	0	7.1	8.4	84.5	100
219 (EU)--V	9.611	2.7	3.5	18.2	75.5	100
220 (EU)--V	9.611	2.7	3.5	18.2	75.5	100
221 A1G)--V	9.72	1	15.7	13.3	70	100
222 (A2G)--V	10.312	0	0	0.6	99.4	100
223 (EU)--V	10.397	2.9	11.1	6.2	79.8	100
224 (EU)--V	10.397	2.9	11.1	6.2	79.8	100
225 (EU)--V	10.456	1	2	4.2	92.8	100
226 (EU)--V	10.456	1	2	4.2	92.8	100
227 (B1G)--V	10.757	0	19.2	7.4	73.3	100
228 (EU)--V	12.242	2	4.3	3.9	89.8	100
229 (EU)--V	12.242	2	4.3	3.9	89.8	100
230 (A2G)--V	12.339	0	0.3	6.9	92.8	100
231 B2G)--V	12.585	0	0.3	0.1	99.6	100
232 (EG)--V	12.801	0	1.5	1.4	97.2	100
233 (EG)--V	12.801	0	1.5	1.4	97.2	100
234 (B2U)--V	13.005	0	0.4	0	99.6	100
235 (A2U)--V	13.109	3.7	0.1	0.7	95.4	100
236 (EU)--V	13.399	0.2	0.3	2.8	96.7	100
237 (EU)--V	13.399	0.2	0.3	2.8	96.7	100
238 (EG)--V	13.649	0	2.3	1.6	96	100
239 (EG)--V	13.649	0	2.3	1.6	96	100
240 (A1G)--V	13.68	0.7	3.1	0.9	95.4	100
241 A2G)--V	13.783	0	0.7	2	97.3	100
242 (B1U)--V	13.958	0	0	4.5	95.5	100
243 (B2G)--V	13.969	0	0.4	1.1	98.5	100
244 (B1G)--V	14.021	0	34	5	60.9	100
245 (EU)--V	14.065	0.1	0.4	0.5	99	100
246 (EU)--V	14.065	0.1	0.4	0.5	99	100
247 (EU)--V	14.314	0	0.8	1.9	97.2	100
248 (EU)--V	14.314	0	0.8	1.9	97.2	100

249 (B2G)--V	14.328	0	0.8	1.8	97.4	100
250 (B1G)--V	14.37	0	2.9	3.1	94	100
251 A2G)--V	14.458	0	0.3	1	98.7	100
252 (B2U)--V	14.471	0	1.3	0.1	98.6	100
253 (A2U)--V	14.589	10.3	1.4	1.4	86.9	100
254 (A1G)--V	14.622	1.9	1.5	15.1	81.5	100
255 (EG)--V	14.764	0	0.5	1.7	97.8	100
256 (EG)--V	14.764	0	0.5	1.7	97.8	100
257 (EU)--V	14.791	0.1	1.4	2.1	96.4	100
258 (EU)--V	14.791	0.1	1.4	2.1	96.4	100
259 (B1G)--V	14.889	0	25.7	1.2	73.1	100
260 (A1U)--V	14.906	0	0	0	100	100
261 A1G)--V	15.32	1	0.1	13.5	85.4	100
262 (EU)--V	15.357	0.2	13.5	16.5	69.9	100
263 (EU)--V	15.357	0.2	13.5	16.5	69.9	100
264 (A2G)--V	15.484	0	1	1.7	97.3	100
265 (B1G)--V	15.562	0	1.8	0.5	97.7	100
266 (EU)--V	15.568	0.2	0.9	0.2	98.7	100
267 (EU)--V	15.568	0.2	0.9	0.2	98.7	100
268 (B2G)--V	15.606	0	0.9	11.6	87.5	100
269 (A1G)--V	15.662	1.9	15.3	2.7	80.1	100
270 (B1U)--V	15.7	0	0	1.1	98.9	100
271 (EG)--V	15.897	0	4.1	0.5	95.3	100
272 (EG)--V	15.897	0	4.1	0.5	95.3	100
273 (A1G)--V	15.914	0.4	22.1	14.1	63.4	100
274 (A2G)--V	15.995	0	0.8	2.9	96.3	100
275 (EU)--V	15.997	1.2	21.7	11.9	65.2	100
276 (EU)--V	15.997	1.2	21.7	11.9	65.2	100
277 (EU)--V	16.32	1.5	3	2.3	93.1	100
278 (EU)--V	16.32	1.5	3	2.3	93.1	100
279 (EU)--V	16.335	1.5	1.9	12	84.5	100
280 (EU)--V	16.335	1.5	1.9	12	84.5	100
281 B2G)--V	16.469	0	0.7	13.9	85.4	100
282 (EG)--V	16.571	0	1.3	3.8	95	100
283 (EG)--V	16.571	0	1.3	3.8	95	100
284 (A2U)--V	16.618	3	1.2	1.3	94.5	100
285 (B2U)--V	16.712	0	1.8	0	98.1	100
286 B1G)--V	16.718	0.1	14.8	7.1	78	100
287 (A1U)--V	16.791	0	0	0	100	100
288 (B1U)--V	17.469	0	0	2.3	97.7	100
289 (EG)--V	17.584	0	0.7	0.3	99.1	100
290 (EG)--V	17.584	0	0.7	0.3	99.1	100
291 A2U)--V	17.771	0.7	0.4	4.2	94.7	100
292 (A1G)--V	17.842	6	22.9	3.8	67.2	100
293 (B2U)--V	19.044	0	1.1	0	98.9	100
294 (EG)--V	19.082	0	1.9	2.1	96	100
295 (EG)--V	19.082	0	1.9	2.1	96	100
296 A1U)--V	19.307	0	0	0	100	100
297 (EU)--V	19.349	5.7	15.3	7.2	71.8	100
298 (EU)--V	19.349	5.7	15.3	7.2	71.8	100
299 (B1U)--V	19.81	0	0	3.5	96.5	100



300 (EG)--V	20.201	0.3	36.6	6.3	56.9	100
301 (EG)--V	20.201	0.3	36.6	6.3	56.9	100
302 (B2G)--V	20.318	0	0.1	3.4	96.5	100
303 (EU)--V	20.561	0.1	1	1.6	97.4	100
304 (EU)--V	20.561	0.1	1	1.6	97.4	100
305 (A1G)--V	20.71	0.1	0.3	0.8	98.8	100
306 A2U)--V	20.971	1.2	12.4	55.1	31.3	100
307 (B2G)--V	21.023	0	2	1.7	96.3	100
308 (A2G)--V	21.249	0	0.3	0.7	99.1	100
309 (EU)--V	21.329	0.1	0.1	1.1	98.7	100
310 (EU)--V	21.329	0.1	0.1	1.1	98.7	100
311 (EG)--V	21.391	0	1.7	0.4	97.9	100
312 (EG)--V	21.391	0	1.7	0.4	97.9	100
313 (A2G)--V	21.699	0	1.5	1.2	97.3	100
314 (EU)--V	21.776	0	0.8	0.5	98.7	100
315 (EU)--V	21.776	0	0.8	0.5	98.7	100
316 B1G)--V	21.81	0	0.9	0.4	98.7	100
317 (B2G)--V	21.976	0	10.3	8.7	80.9	100
318 (B2G)--V	22.377	0	1.2	5.2	93.6	100
319 (A1G)--V	22.403	0.4	8.9	7.3	83.3	100
320 (EU)--V	22.503	0.2	1.8	3.5	94.5	100
321 (EU)--V	22.503	0.2	1.8	3.5	94.5	100
322 (B2U)--V	22.691	0	67.7	0	32.3	100
323 (A2G)--V	22.801	0	0.8	9.8	89.5	100
324 (A1U)--V	22.974	0	0	0	100	100
325 (EU)--V	23.056	0.1	0.6	3.2	96.1	100
326 (EU)--V	23.056	0.1	0.6	3.2	96.1	100
327 (B1G)--V	23.056	0	0.5	0	99.4	100
328 (A1G)--V	23.206	2.5	2.7	26.9	67.9	100
329 (EG)--V	23.522	0.1	14	41.5	44.4	100
330 (EG)--V	23.522	0.1	14	41.5	44.4	100
331 B1U)--V	23.6	0	0	63.1	36.9	100
332 (B1G)--V	23.751	0	20.2	10.3	69.5	100
333 (EU)--V	23.909	0.4	3.6	7.9	88.1	100
334 (EU)--V	23.909	0.4	3.6	7.9	88.1	100
335 (A1G)--V	23.923	0.8	10.1	6.3	82.8	100
336 (EU)--V	24.393	0.3	9	4.9	85.8	100
337 (EU)--V	24.393	0.3	9	4.9	85.8	100
338 (A2G)--V	24.512	0	0	0	100	100
339 (B1G)--V	24.669	0	0.3	0.4	99.3	100
340 (EU)--V	25.021	0.3	0.1	3.7	95.8	100
341 (EU)--V	25.021	0.3	0.1	3.7	95.8	100
342 (A2U)--V	25.539	4.6	42.7	16	36.8	100
343 (B2G)--V	25.549	0	0	0.6	99.3	100
344 (A2G)--V	25.629	0	0	1.7	98.3	100
345 (EU)--V	25.743	0	0.8	2.4	96.7	100
346 (EU)--V	25.743	0	0.8	2.4	96.7	100
347 (B2G)--V	26.133	0	1.2	2.2	96.6	100
348 (B1G)--V	26.323	0	8.3	1.7	90	100
349 (EU)--V	26.493	0.5	7	3.7	88.8	100
350 (EU)--V	26.493	0.5	7	3.7	88.8	100

351 A1G)--V	26.905	0	3.3	3.4	93.2	100
352 (EU)--V	26.919	0	6.3	5.8	87.9	100
353 (EU)--V	26.919	0	6.3	5.8	87.9	100
354 (A1G)--V	27.197	0.2	6	6.2	87.6	100
355 (B2G)--V	27.711	0	7	3.9	89	100
356 (EU)--V	28.112	0	2	2.7	95.2	100
357 (EU)--V	28.112	0	2	2.7	95.2	100
358 (A2G)--V	28.233	0	0.8	0.1	99.1	100
359 (A2G)--V	29.115	0	2.5	2	95.5	100
360 (B1G)--V	29.223	0	1	14.8	84.2	100
361 (EU)--V	29.364	0.1	1.2	0.6	98.1	100
362 (EU)--V	29.364	0.1	1.2	0.6	98.1	100
363 (B2G)--V	29.472	0	0.8	4.5	94.7	100
364 (B1G)--V	29.759	0	5.2	12.5	82.3	100
365 (A1G)--V	30.028	0.9	6.5	3.7	88.9	100
366 (EU)--V	30.17	0.2	5.5	2.9	91.4	100
367 (EU)--V	30.17	0.2	5.5	2.9	91.4	100
368 (B2G)--V	30.503	0	1.3	2.6	96	100
369 (B2U)--V	31.197	0	8	8.4	83.7	100
370 (A1G)--V	31.198	5.5	3.8	0.4	90.3	100
371 (EU)--V	31.408	1	6.8	4.6	87.6	100
372 (EU)--V	31.408	1	6.8	4.6	87.6	100
373 (EG)--V	31.586	0.2	5.3	14.5	80	100
374 (EG)--V	31.586	0.2	5.3	14.5	80	100
375 (A2G)--V	31.604	0	1.6	13.8	84.6	100
376 B1G)--V	32.109	0.3	9.9	9.5	80.3	100
377 (A2U)--V	32.202	0.2	0.8	10.9	88.1	100
378 (EU)--V	32.636	0.2	3.5	8.9	87.4	100
379 (EU)--V	32.636	0.2	3.5	8.9	87.4	100
380 (B2G)--V	32.849	0	1.7	2	96.3	100
381 A1U)--V	33.084	0	19.8	18.3	62	100
382 (EG)--V	33.116	0	8.6	10	81.3	100
383 (EG)--V	33.116	0	8.6	10	81.3	100
384 (B2U)--V	33.199	0	6.3	9.9	83.8	100
385 (EU)--V	33.641	0.2	1.8	13.1	84.9	100
386 (EU)--V	33.641	0.2	1.8	13.1	84.9	100
387 (B1U)--V	34.108	0	5.1	6.6	88.3	100
388 (A2G)--V	34.119	0	0.7	8.2	91.1	100
389 (EG)--V	34.19	0.2	5.2	7	87.6	100
390 (EG)--V	34.19	0.2	5.2	7	87.6	100
391 B1G)--V	34.374	0	0.4	4.5	95.1	100
392 (A1U)--V	34.416	0	3.7	5.6	90.7	100
393 (A2U)--V	34.971	4.2	27	17.6	51.1	100
394 (EG)--V	35.073	2.1	18.6	7.9	71.4	100
395 (EG)--V	35.073	2.1	18.6	7.9	71.4	100
396 A1G)--V	35.116	3.4	5.4	0.1	91.1	100
397 (EU)--V	35.264	0.1	4.1	0.6	95.2	100
398 (EU)--V	35.264	0.1	4.1	0.6	95.2	100
399 (B1G)--V	35.326	0	6	0.2	93.8	100
400 (EU)--V	36.161	0.3	6.8	0.2	92.7	100
401 (EU)--V	36.161	0.3	6.8	0.2	92.7	100

402 (B2U)--V	36.708	0	28.4	0.6	70.9	100
403 (A1G)--V	37.178	0.1	0.4	0	99.5	100
404 (EU)--V	37.427	0.1	1.2	1.5	97.3	100
405 (EU)--V	37.427	0.1	1.2	1.5	97.3	100
406 (EG)--V	37.444	0.2	3.9	6	89.9	100
407 (EG)--V	37.444	0.2	3.9	6	89.9	100
408 (A2G)--V	37.454	0	3	17.3	79.6	100
409 (B2G)--V	37.456	0	0.1	0.4	99.5	100
410 (A2U)--V	37.462	0.5	2	1.9	95.5	100
411 B1G)--V	37.492	0	0.1	1.1	98.8	100
412 (B2U)--V	37.532	0	0.2	0.7	99.1	100
413 (EG)--V	37.791	0.5	12.4	12.1	75	100
414 (EG)--V	37.791	0.5	12.4	12.1	75	100
415 (A2U)--V	38.017	2.3	10.1	0.7	87	100
416 B2U)--V	38.351	0	2.2	0.7	97.1	100
417 (B1U)--V	38.364	0	18.3	24	57.7	100
418 (EG)--V	38.621	0.3	6.4	3.4	89.9	100
419 (EG)--V	38.621	0.3	6.4	3.4	89.9	100
420 (A1U)--V	38.66	0	0	0	100	100
421 B1U)--V	38.72	0	4	5.8	90.1	100
422 (EG)--V	38.74	0.5	13.3	8.3	77.8	100
423 (EG)--V	38.74	0.5	13.3	8.3	77.8	100
424 (EU)--V	39.063	0	1.3	0.7	98	100
425 (EU)--V	39.063	0	1.3	0.7	98	100
426 A2U)--V	39.591	8.1	39.4	6	46.5	100
427 (A2G)--V	39.684	0	4.3	0	95.6	100
428 (A2G)--V	40.664	0	2	4.1	93.9	100
429 (B2G)--V	41.333	0	0.1	1.5	98.4	100
430 (EU)--V	41.389	0.2	3.8	0.1	95.9	100
431 (EU)--V	41.389	0.2	3.8	0.1	95.9	100
432 (A1G)--V	41.687	0.1	40	0.7	59.1	100
433 (EU)--V	42.007	0.8	14.4	2.8	82	100
434 (EU)--V	42.007	0.8	14.4	2.8	82	100
435 (A1G)--V	42.862	0.3	42.9	1.2	55.5	100
436 B1G)--V	43.393	0	32.1	2.5	65.4	100
437 (B2G)--V	44.478	0	0.2	19	80.8	100
438 (EU)--V	44.963	0.8	1	43.1	55.1	100
439 (EU)--V	44.963	0.8	1	43.1	55.1	100
440 (A1G)--V	45.24	1	0.7	52.5	45.7	100
441 B1G)--V	45.729	0	43.8	10.6	45.6	100
442 (EU)--V	46.057	0.1	36.3	4.3	59.2	100
443 (EU)--V	46.057	0.1	36.3	4.3	59.2	100
444 (B1U)--V	46.074	0	1.5	12.3	86.2	100
445 (A1G)--V	46.229	0.6	44.9	3.7	50.8	100
446 (EG)--V	46.389	0	2.5	9.9	87.6	100
447 (EG)--V	46.389	0	2.5	9.9	87.6	100
448 (A1U)--V	46.847	0	3.5	2.6	93.8	100
449 (B1G)--V	47.289	0	53.7	1.3	44.9	100
450 (EU)--V	47.764	0.1	22	2.3	75.5	100
451 (EU)--V	47.764	0.1	22	2.3	75.5	100
452 (B2G)--V	47.788	0	0.1	11.4	88.5	100

453 (A1G)--V	47.872	0.1	20.8	3.9	75.2	100
454 (EU)--V	48.117	0.1	0.7	24	75.2	100
455 (EU)--V	48.117	0.1	0.7	24	75.2	100
456 A2U)--V	48.21	0.5	10.6	25	63.9	100
457 (A2G)--V	48.285	0	0.5	0	99.5	100
458 (A1G)--V	48.639	0.6	18.9	40.7	39.8	100
459 (EU)--V	49.098	0	10.9	1.6	87.5	100
460 (EU)--V	49.098	0	10.9	1.6	87.5	100
461 B1G)--V	49.113	0	31.4	5.1	63.6	100
462 (EG)--V	49.261	0.4	15.9	17.5	66.2	100
463 (EG)--V	49.261	0.4	15.9	17.5	66.2	100
464 (A2G)--V	49.562	0	0	0.1	99.9	100
465 (A1G)--V	50.065	0	10.9	39.2	49.9	100
466 B2G)--V	50.067	0	0	0.9	99.1	100
467 (EU)--V	50.131	0	0.4	0.9	98.7	100
468 (EU)--V	50.131	0	0.4	0.9	98.7	100
469 (B2U)--V	50.294	0	26.2	11.5	62.3	100
470 (EU)--V	50.387	1.8	5.5	21.1	71.6	100
471 (EU)--V	50.387	1.8	5.5	21.1	71.6	100
472 (B1G)--V	50.547	0	13.7	4.7	81.6	100
473 (B1G)--V	50.593	0	13.3	4.9	81.8	100
474 (EU)--V	50.898	2.8	13	9.3	74.9	100
475 (EU)--V	50.898	2.8	13	9.3	74.9	100
476 (EU)--V	51.528	14.2	31.7	0.5	53.5	100
477 (EU)--V	51.528	14.2	31.7	0.5	53.5	100
478 (A1G)--V	51.831	0.5	7.4	12.9	79.2	100
479 (A2G)--V	51.987	0	0.1	0.6	99.3	100
480 (B2G)--V	52.309	0	0.3	8.3	91.4	100
481 B2U)--V	52.53	0	26.8	14.2	58.9	100
482 (EU)--V	52.734	0	3.5	1.3	95.2	100
483 (EU)--V	52.734	0	3.5	1.3	95.2	100
484 (A1G)--V	53.462	0	18.3	14.2	67.5	100
485 (EU)--V	53.474	0.1	6	3.6	90.3	100
486 (EU)--V	53.474	0.1	6	3.6	90.3	100
487 (EG)--V	53.733	1.1	28.4	17.2	53.3	100
488 (EG)--V	53.733	1.1	28.4	17.2	53.3	100
489 (B1G)--V	53.894	0	28.5	4	67.5	100
490 (B1U)--V	54.876	0	2.5	29.1	68.5	100
491 A1U)--V	54.916	0	24.8	11.3	63.9	100
492 (EG)--V	54.945	3.6	4.8	20.3	71.3	100
493 (EG)--V	54.945	3.6	4.8	20.3	71.3	100
494 (A2G)--V	54.964	0	8.8	4.8	86.4	100
495 (A2U)--V	54.983	0.4	5	20.8	73.9	100
496 B2G)--V	55.146	0	0.2	0.2	99.6	100
497 (EU)--V	55.415	0.1	0.8	1.5	97.6	100
498 (EU)--V	55.415	0.1	0.8	1.5	97.6	100
499 (A2G)--V	55.658	0	2.7	2.6	94.7	100
500 (EU)--V	55.804	0	2.3	4.4	93.3	100
501 (EU)--V	55.804	0	2.3	4.4	93.3	100
502 (B1G)--V	56.309	0	5	9.4	85.7	100
503 (B2G)--V	56.477	0	0.3	6	93.7	100

504 (EU)--V	56.692	0.1	0.8	3.3	95.8	100
505 (EU)--V	56.692	0.1	0.8	3.3	95.8	100
506 A1G)--V	56.94	0.7	4.3	0.8	94.1	100
507 (EG)--V	56.991	42.6	14.6	0.9	41.8	100
508 (EG)--V	56.991	42.6	14.6	0.9	41.8	100
509 (B1U)--V	57.513	0	9.9	13.3	76.8	100
510 (EG)--V	57.646	34.5	8.9	4.6	52	100
511 (EG)--V	57.646	34.5	8.9	4.6	52	100
512 (A1U)--V	58.387	0	5.4	4.9	89.8	100
513 (B2U)--V	58.501	0	1.1	0	98.9	100
514 (A2G)--V	58.655	0	0.1	0.3	99.6	100
515 (EU)--V	58.84	0	3.9	6.9	89.2	100
516 (EU)--V	58.84	0	3.9	6.9	89.2	100
517 (EG)--V	59.052	0.2	8.7	0.1	91	100
518 (EG)--V	59.052	0.2	8.7	0.1	91	100
519 (B1U)--V	59.168	0	6.3	1.5	92.2	100
520 (EG)--V	59.335	1.8	1.5	6.3	90.4	100
521 (EG)--V	59.335	1.8	1.5	6.3	90.4	100
522 (A2U)--V	59.431	0.3	29.8	6.1	63.8	100
523 (A2U)--V	59.514	0.1	14	0.7	85.2	100
524 (A1U)--V	59.64	0	0.2	4.8	95	100
525 (A2G)--V	59.769	0	3.1	1.3	95.5	100
526 B2G)--V	59.773	0	0.2	12	87.8	100
527 (EU)--V	60.255	2.1	13.3	16	68.5	100
528 (EU)--V	60.255	2.1	13.3	16	68.5	100
529 (B1G)--V	60.521	0	36.1	16.6	47.4	100
530 (B2U)--V	60.537	0	2.5	1.2	96.4	100
531 (EG)--V	60.554	0	8.6	4.5	86.8	100
532 (EG)--V	60.554	0	8.6	4.5	86.8	100
533 (A1G)--V	61.527	0.1	1.2	17.6	81.1	100
534 (B2G)--V	61.909	5.5	5.2	4.3	85	100
535 (B1U)--V	62.349	0	18.1	1.7	80.2	100
536 (EU)--V	62.954	0.1	1.9	25.7	72.3	100
537 (EU)--V	62.954	0.1	1.9	25.7	72.3	100
538 (EG)--V	63.396	0.7	15.4	8.7	75.3	100
539 (EG)--V	63.396	0.7	15.4	8.7	75.3	100
540 (A2G)--V	63.597	0	0.1	0	99.9	100
541 (EU)--V	63.972	0	0.2	0.6	99.2	100
542 (EU)--V	63.972	0	0.2	0.6	99.2	100
543 (B1G)--V	64.268	0	1.7	0.1	98.2	100
544 (B2G)--V	64.28	0	2.5	25	72.4	100
545 (B2G)--V	64.751	0.4	3.5	3.2	92.8	100
546 A1U)--V	65.583	0	2.6	6.7	90.7	100
547 (A1G)--V	65.731	2.1	16.6	1.6	79.7	100
548 (A2U)--V	65.735	0.2	8.7	19.2	72	100
549 (EU)--V	66.026	0.2	8.8	11.1	79.9	100
550 (EU)--V	66.026	0.2	8.8	11.1	79.9	100
551 (EG)--V	66.795	0	7.5	10	82.5	100
552 (EG)--V	66.795	0	7.5	10	82.5	100
553 (A1U)--V	67.868	0	13.5	12.4	74.1	100
554 (B1U)--V	67.994	0	12.2	8.3	79.5	100

555 (B1G)--V	69.156	0.7	56.1	5	38.2	100
556 A1G)--V	69.268	2.7	18.1	35.8	43.4	100
557 (A2G)--V	69.572	0	0.7	0.3	99	100
558 (EG)--V	69.779	0.3	7.2	10.8	81.7	100
559 (EG)--V	69.779	0.3	7.2	10.8	81.7	100
560 (EU)--V	69.938	0	0.2	0.4	99.3	100
561 (EU)--V	69.938	0	0.2	0.4	99.3	100
562 (B2G)--V	69.943	0	0.3	0.1	99.6	100
563 (EU)--V	70.194	0.1	17.8	12.1	70	100
564 (EU)--V	70.194	0.1	17.8	12.1	70	100
565 (B1G)--V	70.415	0	0.3	3.6	96	100
566 (EU)--V	70.568	0.1	25.2	26.9	47.8	100
567 (EU)--V	70.568	0.1	25.2	26.9	47.8	100
568 (B1U)--V	70.622	0	0.2	4.2	95.7	100
569 (A1G)--V	70.657	2.3	11.5	23.8	62.4	100
570 (A2G)--V	70.724	0	2.1	1.7	96.2	100
571 (EU)--V	70.917	0	10	8.3	81.7	100
572 (EU)--V	70.917	0	10	8.3	81.7	100
573 (B1G)--V	71.064	0	28.4	3.4	68.3	100
574 (A1G)--V	71.526	6.3	6.9	0.8	86	100
575 (B2U)--V	71.732	0	16	30.7	53.3	100
576 A1U)--V	71.882	0	5.5	16.7	77.8	100
577 (EG)--V	71.931	0.2	9.9	22.1	67.8	100
578 (EG)--V	71.931	0.2	9.9	22.1	67.8	100
579 (B1G)--V	72.108	0.2	27.5	4.1	68.2	100
580 (EU)--V	72.158	0.1	41.1	14.4	44.5	100
581 (EU)--V	72.158	0.1	41.1	14.4	44.5	100
582 (A1G)--V	72.386	0.1	53.9	20.2	25.7	100
583 (B2G)--V	73.146	0	0.2	7.2	92.6	100
584 (B2G)--V	73.505	0.1	3.9	20.9	75.1	100
585 (EU)--V	73.887	0	2.1	6.6	91.3	100
586 (EU)--V	73.887	0	2.1	6.6	91.3	100
587 (A2G)--V	74.238	0	0.9	6.5	92.6	100
588 (B1G)--V	74.298	1.2	51.7	4.5	42.6	100
589 (B2G)--V	74.71	0	0.1	0.3	99.6	100
590 (EU)--V	75.448	0	2.6	4.7	92.7	100
591 (EU)--V	75.448	0	2.6	4.7	92.7	100
592 (EU)--V	77.007	0.1	7.4	4.8	87.7	100
593 (EU)--V	77.007	0.1	7.4	4.8	87.7	100
594 (A2G)--V	77.186	0	1.2	2.6	96.2	100
595 (A1G)--V	77.439	0.3	21.2	25.3	53.2	100
596 (EU)--V	77.505	0.4	6.1	5.2	88.3	100
597 (EU)--V	77.505	0.4	6.1	5.2	88.3	100
598 (B2G)--V	79.07	0	0.1	7.9	92	100
599 (B1G)--V	79.104	0.8	6.8	6	86.5	100
600 (A2G)--V	80.082	0	0.4	0	99.6	100
601 A1G)--V	80.46	0.5	3.9	4.6	91	100
602 (EU)--V	80.656	0.1	9.8	10.8	79.4	100
603 (EU)--V	80.656	0.1	9.8	10.8	79.4	100
604 (A2G)--V	81.361	0	15.1	4.5	80.4	100
605 (B2G)--V	82.497	0	2.3	2.5	95.2	100

606 (EU)--V	82.968	0	1	5.1	93.9	100
607 (EU)--V	82.968	0	1	5.1	93.9	100
608 (EU)--V	85.348	0.2	7.4	19.7	72.8	100
609 (EU)--V	85.348	0.2	7.4	19.7	72.8	100
610 (B1G)--V	86.669	0.8	5.2	25.8	68.2	100
611 A1G)--V	88.551	0.4	4.2	55.2	40.3	100
612 (B2G)--V	89.041	0	1	1.8	97.3	100
613 (EU)--V	90.218	0	1.4	2.9	95.6	100
614 (EU)--V	90.218	0	1.4	2.9	95.6	100
615 (A2G)--V	90.936	0	6.4	11.6	82	100
616 A2G)--V	91.043	0	2.6	2.5	94.8	100
617 (EU)--V	92.953	0	5.5	4.4	90.1	100
618 (EU)--V	92.953	0	5.5	4.4	90.1	100
619 (B2G)--V	93.629	0	4	3	93	100

### B3LYP Exchange Correlation Functional

Orbital	Index	E, eV	Zn	NZn	Nmeso	Pc	Total	
	1 A1G)--O	-9449.16		100	0	0	0	100
	2 (A1G)--O	-1148.77		100	0	0	0	100
	3 (A2U)--O	-1012.4		0	0	0	0	100
	4 (EU)--O	-1012.21		100	0	0	0	100
	5 (EU)--O	-1012.21		100	0	0	0	100
	6 B1G)--O	-390.386		0	99.8	0	0.2	100
	7 (EU)--O	-390.386		0	99.8	0	0.1	100
	8 (EU)--O	-390.386		0	99.8	0	0.1	100
	9 (A1G)--O	-390.386		0	99.9	0	0.1	100
	10 (B2G)--O	-390.158		0	0	99.8	0.2	100
	11 (EU)--O	-390.158		0	0	99.8	0.2	100
	12 (EU)--O	-390.158		0	0	99.8	0.2	100
	13 (A1G)--O	-390.158		0	0	99.8	0.1	100
	14 (B2G)--O	-279.242		0	0	0.1	99.8	100
	15 (EU)--O	-279.242		0	0	0.1	99.9	100
	16 (EU)--O	-279.242		0	0	0.1	99.9	100
	17 (A1G)--O	-279.241		0	0	0	100	100
	18 (A2G)--O	-279.241		0	0	0	100	100
	19 (EU)--O	-279.241		0	0	0	100	100
	20 (EU)--O	-279.241		0	0	0	100	100
	21 B1G)--O	-279.24		0	0	0	100	100
	22 (EU)--O	-277.381		0	0	0	100	100
	23 (EU)--O	-277.381		0	0	0	100	100
	24 (B1G)--O	-277.381		0	0	0	100	100
	25 (A1G)--O	-277.381		0	0	0	100	100
	26 A2G)--O	-277.38		0	0	0	100	100
	27 (EU)--O	-277.38		0	0	0	100	100
	28 (EU)--O	-277.38		0	0	0	100	100
	29 (B2G)--O	-277.38		0	0	0	100	100
	30 (EU)--O	-277.368		0	0	0	100	100
	31 (EU)--O	-277.368		0	0	0	100	100

32 (A1G)--O	-277.367	0	0	0	100	100
33 (B1G)--O	-277.367	0	0	0	100	100
34 (EU)--O	-277.361	0	0	0	100	100
35 (EU)--O	-277.361	0	0	0	100	100
36 B1G)--O	-277.361	0	0	0	100	100
37 (A1G)--O	-277.361	0	0	0	100	100
38 (A2G)--O	-277.357	0	0	0	100	100
39 (EU)--O	-277.357	0	0	0	100	100
40 (EU)--O	-277.357	0	0	0	100	100
41 B2G)--O	-277.357	0	0	0	100	100
42 (B2G)--O	-277.353	0	0	0	100	100
43 (EU)--O	-277.353	0	0	0	100	100
44 (EU)--O	-277.353	0	0	0	100	100
45 (A2G)--O	-277.353	0	0	0	100	100
46 A1G)--O	-130.634	15.9	0	0	0	100
47 (A2U)--O	-87.03	0	0	0	0	100
48 (EU)--O	-86.755	11.3	0	0	0	100
49 (EU)--O	-86.755	11.3	0	0	0	100
50 (A1G)--O	-27.405	0	39.3	25.6	34.7	100
51 (EU)--O	-27.013	0	38.3	25.5	36	100
52 (EU)--O	-27.013	0	38.3	25.5	36	100
53 (B1G)--O	-26.241	0	58.9	0.8	40.1	100
54 (B2G)--O	-25.68	0	1.7	69.9	28.4	100
55 (EU)--O	-24.549	0	18.2	49.7	32.1	100
56 (EU)--O	-24.549	0	18.2	49.7	32.1	100
57 (A1G)--O	-23.693	0	16.7	49.4	33.8	100
58 (A1G)--O	-23.246	0	22.6	8.6	68.5	100
59 (EU)--O	-23.23	0	14.6	1.2	84.1	100
60 (EU)--O	-23.23	0	14.6	1.2	84.1	100
61 B1G)--O	-23.215	0	13.1	0	86.8	100
62 (A2G)--O	-21.048	0	2.7	6.3	91	100
63 (A1G)--O	-20.722	0	12.4	0.3	86.7	100
64 (EU)--O	-20.694	0	13.5	3.9	82.6	100
65 (EU)--O	-20.694	0	13.5	3.9	82.6	100
66 (EU)--O	-20.58	0	4.6	1.2	94.1	100
67 (EU)--O	-20.58	0	4.6	1.2	94.1	100
68 (B1G)--O	-20.57	0	18.9	0.6	80	100
69 (B2G)--O	-20.503	0	0	1.8	98.2	100
70 (A2G)--O	-19.586	0	5.8	9	85.2	100
71 (EU)--O	-18.859	0	7.2	18.6	74.1	100
72 (EU)--O	-18.859	0	7.2	18.6	74.1	100
73 (B1G)--O	-17.409	0	12.6	18.1	68.1	100
74 (A1G)--O	-17.303	0.1	11.7	0.4	86	100
75 (EU)--O	-17.131	0	10.9	0.3	88.5	100
76 (EU)--O	-17.131	0	10.9	0.3	88.5	100
77 (B2G)--O	-16.985	0	3.1	13.2	83.7	100
78 (B1G)--O	-16.842	0	4.2	12.1	83	100
79 (EU)--O	-16.19	0	5.8	3.7	90.5	100
80 (EU)--O	-16.19	0	5.8	3.7	90.5	100
81 B2G)--O	-16.08	0	31.3	22.5	43.9	100
82 (A2G)--O	-15.937	0	5.9	1.8	92.3	100



83 (A1G)--O	-15.099	0.1	9.2	1.4	85.4	100
84 (EU)--O	-14.914	0	18.1	12.6	69.3	100
85 (EU)--O	-14.914	0	18.1	12.6	69.3	100
86 B1G)--O	-14.511	0	14.9	5.2	65.7	100
87 (EU)--O	-14.475	0	15.1	19.6	65	100
88 (EU)--O	-14.475	0	15.1	19.6	65	100
89 (B2G)--O	-13.632	0	2.3	1.7	93.7	100
90 (A2G)--O	-13.598	0	25.9	15	59.1	100
91 B1G)--O	-13.353	0	13.7	0.5	35.3	100
92 (A1G)--O	-13.316	0.1	20	0.9	43.5	100
93 (EU)--O	-13.102	0	2.6	4.3	93.1	100
94 (EU)--O	-13.102	0	2.6	4.3	93.1	100
95 (EU)--O	-12.643	0	13.6	1	84.8	100
96 (EU)--O	-12.643	0	13.6	1	84.8	100
97 (EG)--O	-12.617	0	11.8	2.8	9.7	100
98 (EG)--O	-12.617	0	11.8	2.8	9.7	100
99 (A2G)--O	-12.584	0	0.5	7.7	91.8	100
100 (A2U)--O	-12.552	0	26.1	18.3	55.1	100
101 A1G)--O	-12.309	0	6.5	3.1	45.7	100
102 (B1G)--O	-12.241	0	8	1.2	74.6	100
103 (B2G)--O	-12.043	0	4.7	0.5	48.4	100
104 (A1G)--O	-11.982	0	1.5	3.6	79.4	100
105 (EU)--O	-11.96	0	1.1	1.5	97.3	100
106 (EU)--O	-11.96	0	1.1	1.5	97.3	100
107 (B2G)--O	-11.939	0	1.7	1.6	76.5	100
108 (EG)--O	-11.831	0	7.2	9.9	35.4	100
109 (EG)--O	-11.831	0	7.2	9.9	35.4	100
110 (A2G)--O	-11.667	0	0.6	4	95.4	100
111 (EU)--O	-11.566	0	5.5	4.6	89.7	100
112 (EU)--O	-11.566	0	5.5	4.6	89.7	100
113 (B2U)--O	-11.321	0	27.5	0	72.5	100
114 (B1G)--O	-11.25	0	0.8	3.9	86.2	100
115 (A1G)--O	-10.782	0.5	19.5	4.3	36.2	100
116 B1U)--O	-10.393	0	0	51.6	48.4	100
117 (B2G)--O	-10.101	0	0.1	1.7	97.8	100
118 (EU)--O	-10.019	0	1.7	2.3	95.9	100
119 (EU)--O	-10.019	0	1.7	2.3	95.9	100
120 (EG)--O	-9.85	0	2.7	13.7	82.7	100
121 (EG)--O	-9.85	0	2.7	13.7	82.7	100
122 (A2U)--O	-9.829	0	7.5	3.7	88.4	100
123 (A2G)--O	-9.81	0	1.9	1.1	96.9	100
124 (EU)--O	-9.659	0.1	32.5	2.8	60.8	100
125 (EU)--O	-9.659	0.1	32.5	2.8	60.8	100
126 A1G)--O	-9.639	0	1.7	3.2	95.2	100
127 (B2U)--O	-9.407	0	27.3	0	72.7	100
128 (B1G)--O	-9.284	0	1.1	2.9	94.5	100
129 (EU)--O	-9.249	0.1	18.2	7.1	72.2	100
130 (EU)--O	-9.249	0.1	18.2	7.1	72.2	100
131 (EG)--O	-8.636	0	22.1	21.9	54.3	100
132 (EG)--O	-8.636	0	22.1	21.9	54.3	100
133 (A1G)--O	-8.252	0	17.7	55.2	26.8	100

134 (EU)--O	-7.512	0	18	50.2	31.6	100
135 (EU)--O	-7.512	0	18	50.2	31.6	100
136 A1U)--O	-7.501	0	0	0	100	100
137 (A2U)--O	-7.064	0	46.2	20.4	30.6	100
138 (B2G)--O	-7.028	0	12.3	61.6	25.6	100
139 (B1U)--O	-6.974	0	0	5.2	94.8	100
140 (EG)--O	-6.942	0	0.7	10.1	89.2	100
141 (EG)--O	-6.942	0	0.7	10.1	89.2	100
142 (A2U)--O	-6.772	0	6.2	39.7	53.9	100
143 (EG)--O	-6.747	0	27.7	1.3	69.7	100
144 (EG)--O	-6.747	0	27.7	1.3	69.7	100
145 (B2U)--O	-6.716	0	25.2	0	74.8	100
146 B1G)--O	-6.652	0	53.8	0.9	25.1	100
147 (A1U)--O	-4.936	0	0.1	0.1	99.8	100
148 (EG)--V	-2.749	0	13.3	19	67.4	100
149 (EG)--V	-2.749	0	13.3	19	67.4	100
150 (B1U)--V	-1.066	0	0	23.8	76.2	100
151 B2U)--V	-0.823	0	19	0	81	100
152 (A2U)--V	-0.69	0	0.6	5.7	85	100
153 (EG)--V	-0.516	0	5.2	3.6	91.1	100
154 (EG)--V	-0.516	0	5.2	3.6	91.1	100
155 (A1U)--V	0.749	0	0	0	100	100
156 A2U)--V	0.756	0	8.9	1.1	25.9	100
157 (EG)--V	0.824	0	1.8	1	97.2	100
158 (EG)--V	0.824	0	1.8	1	97.2	100
159 (A1G)--V	0.962	0	13.7	0.2	9.3	100
160 (B2U)--V	1.456	0	19.4	0.1	80.5	100
161 B1U)--V	1.7	0	0.1	19.1	80.8	100
162 (EU)--V	2.59	0	5.5	1.9	35.6	100
163 (EU)--V	2.59	0	5.5	1.9	35.6	100
164 (A1G)--V	2.66	0	0	1.4	98.3	100
165 (EU)--V	2.817	0	1.4	0.3	79.9	100
166 (EU)--V	2.817	0	1.4	0.3	79.9	100
167 (B1G)--V	2.854	0	0	0.1	99.9	100
168 (EG)--V	3.112	0	14.3	16	69.6	100
169 (EG)--V	3.112	0	14.3	16	69.6	100
170 (A2U)--V	3.604	0	12.9	15.2	35.5	100
171 B2G)--V	3.66	0	0.8	0.1	99.1	100
172 (EU)--V	3.875	0	0.9	0.2	98.8	100
173 (EU)--V	3.875	0	0.9	0.2	98.8	100
174 (A1G)--V	4.036	0.1	0.4	9.3	65.7	100
175 (A2G)--V	4.141	0	0.6	0.1	99.3	100
176 (EU)--V	4.562	0	0.1	2.6	96.7	100
177 (EU)--V	4.562	0	0.1	2.6	96.7	100
178 (B2G)--V	4.608	0	0	3.6	96.4	100
179 (A1U)--V	4.854	0	0	0	100	100
180 (A1G)--V	4.874	0.1	1.3	0.5	61.7	100
181 B1G)--V	5.001	0	3	0.1	96.9	100
182 (EU)--V	5.002	0	1.2	0.1	98.3	100
183 (EU)--V	5.002	0	1.2	0.1	98.3	100
184 (EG)--V	5.041	0	0.9	4.1	95	100

185 (EG)--V	5.041	0	0.9	4.1	95	100
186 B1U)--V	5.053	0	0	4.6	95.4	100
187 (A2G)--V	5.136	0	0	0	99.9	100
188 (EU)--V	5.886	0	10.9	5.4	78.3	100
189 (EU)--V	5.886	0	10.9	5.4	78.3	100
190 (B2G)--V	5.916	0	3	15.3	81.7	100
191 A1G)--V	6.234	0	0.6	1.3	98.1	100
192 (B1G)--V	6.25	0	31.5	3.4	65.2	100
193 (A2U)--V	6.499	0	4.6	2	10.8	100
194 (EU)--V	6.762	0	0.7	1.8	97.4	100
195 (EU)--V	6.762	0	0.7	1.8	97.4	100
196 A2G)--V	6.845	0	6.1	0.6	93.3	100
197 (B2G)--V	7.074	0	0.4	11.8	87.8	100
198 (EU)--V	7.094	0	0.2	5.8	93.3	100
199 (EU)--V	7.094	0	0.2	5.8	93.3	100
200 (A2G)--V	7.352	0	0.2	0	99.8	100
201 B1G)--V	7.423	0	1.8	0	98.2	100
202 (A1G)--V	7.75	0	9	23	60.4	100
203 (EU)--V	7.759	0	4.4	2.2	92.2	100
204 (EU)--V	7.759	0	4.4	2.2	92.2	100
205 (EU)--V	8.175	0	8.5	3	87.7	100
206 (EU)--V	8.175	0	8.5	3	87.7	100
207 (A1G)--V	8.218	0	0.5	2.4	92.8	100
208 (B1G)--V	8.878	0	0.5	0.1	99.4	100
209 (B2G)--V	8.898	0	1	5.1	93.9	100
210 (EU)--V	9.153	0	2.4	14.2	83.1	100
211 (EU)--V	9.153	0	2.4	14.2	83.1	100
212 (A1G)--V	9.389	0	2.2	2.5	95	100
213 (EU)--V	9.431	0	4.9	1.7	91.9	100
214 (EU)--V	9.431	0	4.9	1.7	91.9	100
215 (B2G)--V	9.7	0	4.1	24.1	71.8	100
216 B1G)--V	9.956	0	4.3	0.1	95.6	100
217 (B2G)--V	10.321	0	1.3	12.4	86.3	100
218 (A1G)--V	10.667	0	17.3	12.8	68.9	100
219 (EU)--V	10.673	0	3.9	17	76.6	100
220 (EU)--V	10.673	0	3.9	17	76.6	100
221 A2G)--V	10.773	0	6.7	8.6	84.7	100
222 (A2G)--V	11.576	0	0	0.8	99.2	100
223 (EU)--V	11.579	0	10.9	8.8	77.5	100
224 (EU)--V	11.579	0	10.9	8.8	77.5	100
225 (B1G)--V	11.693	0	19.5	8.3	72.2	100
226 (EU)--V	11.742	0	1.3	3.5	94.6	100
227 (EU)--V	11.742	0	1.3	3.5	94.6	100
228 (EU)--V	13.518	0	3.7	3.6	90.7	100
229 (EU)--V	13.518	0	3.7	3.6	90.7	100
230 (A2G)--V	13.74	0	0.2	5.9	93.8	100
231 (EG)--V	13.783	0	1.4	1.4	97.2	100
232 (EG)--V	13.783	0	1.4	1.4	97.2	100
233 (B2G)--V	13.909	0	0.3	0	99.7	100
234 (B2U)--V	14.004	0	0.4	0	99.6	100
235 (A2U)--V	14.112	0	0.2	0.7	95.4	100

236 (EU)--V	14.619	0	0.5	2.7	96.6	100
237 (EU)--V	14.619	0	0.5	2.7	96.6	100
238 (EG)--V	14.659	0	2	1.6	96.4	100
239 (EG)--V	14.659	0	2	1.6	96.4	100
240 (A1G)--V	14.823	0	4.6	1	93.7	100
241 A2G)--V	14.936	0	0.9	2.8	96.3	100
242 (B1U)--V	14.938	0	0	4.2	95.8	100
243 (B1G)--V	15.004	0	34.1	5	60.8	100
244 (B2G)--V	15.197	0	0.4	1.3	98.4	100
245 (EU)--V	15.304	0	0.4	0.4	99.1	100
246 (EU)--V	15.304	0	0.4	0.4	99.1	100
247 (EU)--V	15.477	0	0.6	1.4	98	100
248 (EU)--V	15.477	0	0.6	1.4	98	100
249 (B2U)--V	15.48	0	1.3	0.1	98.6	100
250 (B1G)--V	15.493	0	1.1	1.8	97.1	100
251 A2U)--V	15.579	0	1.5	1.4	87.5	100
252 (B2G)--V	15.668	0	0.9	1.6	97.5	100
253 (A2G)--V	15.72	0	0.3	0.9	98.8	100
254 (A1G)--V	15.75	0	1.4	13.6	83.3	100
255 (EG)--V	15.769	0	0.5	1.5	98	100
256 (EG)--V	15.769	0	0.5	1.5	98	100
257 (A1U)--V	15.907	0	0	0	100	100
258 (EU)--V	15.943	0	1	1.3	97.6	100
259 (EU)--V	15.943	0	1	1.3	97.6	100
260 (B1G)--V	16.021	0	25.4	1.2	73.4	100
261 (EU)--V	16.525	0	15.2	15.8	68.8	100
262 (EU)--V	16.525	0	15.2	15.8	68.8	100
263 (A1G)--V	16.532	0	0.1	12.4	86.7	100
264 (A2G)--V	16.705	0	0.8	1.1	98.1	100
265 (B1U)--V	16.723	0	0	1.1	98.9	100
266 B1G)--V	16.723	0	0.6	0.8	98.6	100
267 (EU)--V	16.735	0	1	0.3	98.6	100
268 (EU)--V	16.735	0	1	0.3	98.6	100
269 (B2G)--V	16.792	0	0.8	8.8	90.4	100
270 (A1G)--V	16.86	0	22.5	6	70.5	100
271 (EG)--V	16.951	0	3.4	0.6	96	100
272 (EG)--V	16.951	0	3.4	0.6	96	100
273 (A1G)--V	17.077	0	17.3	20.8	61.5	100
274 (EU)--V	17.148	0	23.3	11	64.6	100
275 (EU)--V	17.148	0	23.3	11	64.6	100
276 A2G)--V	17.422	0	1	3.1	95.9	100
277 (EG)--V	17.667	0	1.1	3.3	95.6	100
278 (EG)--V	17.667	0	1.1	3.3	95.6	100
279 (A2U)--V	17.684	0	1.1	1.2	94.8	100
280 (EU)--V	17.738	0	3.1	1.3	93.8	100
281 (EU)--V	17.738	0	3.1	1.3	93.8	100
282 (B2U)--V	17.804	0	1.6	0	98.4	100
283 (EU)--V	17.853	0	2	13	83.7	100
284 (EU)--V	17.853	0	2	13	83.7	100
285 (A1U)--V	17.858	0	0	0	100	100
286 B2G)--V	17.925	0	0.6	13.8	85.5	100

287 (B1G)--V	18.338	0	12	9.1	78.8	100
288 (B1U)--V	18.569	0	0	2.2	97.8	100
289 (EG)--V	18.694	0	0.5	0.3	99.2	100
290 (EG)--V	18.694	0	0.5	0.3	99.2	100
291 A2U)--V	18.892	0	0.4	3.4	95.6	100
292 (A1G)--V	19.215	0	22.1	4.3	67.8	100
293 (B2U)--V	20.143	0	1	0	99	100
294 (EG)--V	20.18	0	1.1	1.5	97.3	100
295 (EG)--V	20.18	0	1.1	1.5	97.3	100
296 A1U)--V	20.362	0	0	0	100	100
297 (EU)--V	20.608	0	15.4	7.1	72.1	100
298 (EU)--V	20.608	0	15.4	7.1	72.1	100
299 (B1U)--V	20.947	0	0	3.3	96.7	100
300 (EG)--V	21.508	0	33.5	6.7	59.5	100
301 (EG)--V	21.508	0	33.5	6.7	59.5	100
302 (B2G)--V	21.675	0	0.3	3	96.8	100
303 (EU)--V	21.848	0	1.1	1.6	97.2	100
304 (EU)--V	21.848	0	1.1	1.6	97.2	100
305 (A1G)--V	21.97	0	0.3	0.8	98.8	100
306 A2U)--V	22.325	0	11.9	57.3	29.7	100
307 (B2G)--V	22.333	0	1.6	1.6	96.8	100
308 (A2G)--V	22.539	0	0.3	0.9	98.8	100
309 (EG)--V	22.58	0	2.7	0.6	96.7	100
310 (EG)--V	22.58	0	2.7	0.6	96.7	100
311 (EU)--V	22.607	0	0.1	1.1	98.8	100
312 (EU)--V	22.607	0	0.1	1.1	98.8	100
313 (A2G)--V	22.893	0	1.6	0.9	97.5	100
314 (EU)--V	23.026	0	0.9	0.3	98.8	100
315 (EU)--V	23.026	0	0.9	0.3	98.8	100
316 B1G)--V	23.073	0	0.9	0.4	98.6	100
317 (B2G)--V	23.398	0	9.2	10.4	80.3	100
318 (A1G)--V	23.57	0	9.4	7.6	82.5	100
319 (B2G)--V	23.598	0	2.7	3.2	94	100
320 (EU)--V	23.718	0	2	3.6	94.2	100
321 (EU)--V	23.718	0	2	3.6	94.2	100
322 (A2G)--V	24.109	0	0.6	9.2	90.2	100
323 (A1U)--V	24.129	0	0	0	100	100
324 (B2U)--V	24.162	0	69.1	0	30.9	100
325 (B1G)--V	24.252	0	0.2	0.2	99.6	100
326 (EU)--V	24.255	0	0.6	3.4	95.9	100
327 (EU)--V	24.255	0	0.6	3.4	95.9	100
328 (A1G)--V	24.474	0	2.1	24.7	71	100
329 (EG)--V	24.869	0	14.6	41.6	43.6	100
330 (EG)--V	24.869	0	14.6	41.6	43.6	100
331 B1U)--V	24.908	0	0	64.3	35.7	100
332 (B1G)--V	25.069	0	20	10.7	69.3	100
333 (A1G)--V	25.14	0	10.5	6.7	81.9	100
334 (EU)--V	25.258	0	3.5	7.3	89	100
335 (EU)--V	25.258	0	3.5	7.3	89	100
336 (EU)--V	25.625	0	9.4	5.1	85.1	100
337 (EU)--V	25.625	0	9.4	5.1	85.1	100

338 (A2G)--V	25.773	0	0	0	99.9	100
339 (B1G)--V	25.913	0	0.2	0.2	99.6	100
340 (EU)--V	26.292	0	0.2	3.7	95.8	100
341 (EU)--V	26.292	0	0.2	3.7	95.8	100
342 (B2G)--V	26.787	0	0.1	0.8	99.2	100
343 (A2G)--V	26.976	0	0	1.7	98.2	100
344 (A2U)--V	26.994	0	43.4	15.9	36.1	100
345 (EU)--V	27.043	0	1.1	2.7	96.2	100
346 (EU)--V	27.043	0	1.1	2.7	96.2	100
347 (B2G)--V	27.396	0	1.1	2.1	96.8	100
348 (B1G)--V	27.561	0	8.2	2.3	89.6	100
349 (EU)--V	27.769	0	7	3.8	88.8	100
350 (EU)--V	27.769	0	7	3.8	88.8	100
351 (EU)--V	28.141	0	5.8	5.7	88.5	100
352 (EU)--V	28.141	0	5.8	5.7	88.5	100
353 (A1G)--V	28.163	0	3.5	3.5	93	100
354 (A1G)--V	28.52	0	5.8	6.5	87.6	100
355 (B2G)--V	28.925	0	7	4	89	100
356 (EU)--V	29.395	0	2.4	3	94.6	100
357 (EU)--V	29.395	0	2.4	3	94.6	100
358 (A2G)--V	29.48	0	0.8	0.2	99	100
359 (A2G)--V	30.44	0	2.9	2.4	94.7	100
360 (B1G)--V	30.615	0	1.1	15.5	83.4	100
361 (EU)--V	30.715	0	0.9	0.8	98.2	100
362 (EU)--V	30.715	0	0.9	0.8	98.2	100
363 (B2G)--V	30.853	0	0.8	4.3	94.9	100
364 (B1G)--V	31.113	0	4.9	12	83	100
365 (A1G)--V	31.412	0	6.3	3.8	89.1	100
366 (EU)--V	31.528	0	5.7	3.4	90.7	100
367 (EU)--V	31.528	0	5.7	3.4	90.7	100
368 (B2G)--V	31.873	0	1.4	3.9	94.7	100
369 (A1G)--V	32.668	0	3.5	0.4	91.1	100
370 (EU)--V	32.823	0	6.1	4.8	88.1	100
371 (EU)--V	32.823	0	6.1	4.8	88.1	100
372 (B2U)--V	32.916	0	7.8	8.2	84	100
373 (A2G)--V	33.06	0	1.1	14.4	84.5	100
374 (EG)--V	33.308	0	5.4	14	80.5	100
375 (EG)--V	33.308	0	5.4	14	80.5	100
376 (B1G)--V	33.848	0	13.6	8.2	77.9	100
377 (A2U)--V	33.927	0	0.9	10.6	88.4	100
378 (EU)--V	33.927	0	3.7	9.6	86.5	100
379 (EU)--V	33.927	0	3.7	9.6	86.5	100
380 (B2G)--V	34.23	0	1.7	1.9	96.4	100
381 (A1U)--V	34.881	0	20.2	18.1	61.7	100
382 (EG)--V	34.885	0	8.8	9.8	81.3	100
383 (EG)--V	34.885	0	8.8	9.8	81.3	100
384 (B2U)--V	34.969	0	6.5	9.8	83.7	100
385 (EU)--V	35.032	0	1.6	12.3	85.9	100
386 (EU)--V	35.032	0	1.6	12.3	85.9	100
387 (A2G)--V	35.378	0	0.8	8.6	90.6	100
388 (B1U)--V	35.877	0	5.3	6.8	88	100

389 (B1G)--V	35.923	0	0.4	4.3	95.3	100
390 (EG)--V	35.978	0	5.3	7.3	87.3	100
391 (EG)--V	35.978	0	5.3	7.3	87.3	100
392 (A1U)--V	36.218	0	3.5	5.8	90.6	100
393 (A2U)--V	36.673	0	27	17.2	51.6	100
394 (A1G)--V	36.699	0	5.7	0.1	90.7	100
395 (EU)--V	36.77	0	3.6	0.6	95.7	100
396 (EU)--V	36.77	0	3.6	0.6	95.7	100
397 (B1G)--V	36.782	0	6	0.2	93.8	100
398 (EG)--V	36.85	0	18.6	7.8	71.6	100
399 (EG)--V	36.85	0	18.6	7.8	71.6	100
400 (EU)--V	37.603	0	6.7	0.2	92.9	100
401 (EU)--V	37.603	0	6.7	0.2	92.9	100
402 (B2U)--V	38.483	0	28.1	0.7	71.2	100
403 (A1G)--V	38.595	0	0.4	0	99.5	100
404 (A2G)--V	38.847	0	3.1	17.5	79.5	100
405 (EU)--V	38.852	0	1.2	1.6	97.2	100
406 (EU)--V	38.852	0	1.2	1.6	97.2	100
407 (B2G)--V	38.875	0	0.1	0.4	99.5	100
408 (B1G)--V	38.915	0	0.1	1.2	98.7	100
409 (EG)--V	39.295	0	3.8	5.6	90.5	100
410 (EG)--V	39.295	0	3.8	5.6	90.5	100
411 A2U)--V	39.309	0	2	1.9	95.5	100
412 (B2U)--V	39.384	0	0.2	0.7	99.1	100
413 (EG)--V	39.648	0	12.3	11.8	75.5	100
414 (EG)--V	39.648	0	12.3	11.8	75.5	100
415 (A2U)--V	39.863	0	9.9	0.8	87	100
416 B2U)--V	40.23	0	2.3	0.7	97	100
417 (B1U)--V	40.254	0	18	22.9	59	100
418 (EG)--V	40.504	0	5.2	2.6	91.9	100
419 (EG)--V	40.504	0	5.2	2.6	91.9	100
420 (A1U)--V	40.539	0	0	0	100	100
421 (EU)--V	40.549	0	1.4	0.8	97.9	100
422 (EU)--V	40.549	0	1.4	0.8	97.9	100
423 (B1U)--V	40.606	0	4.7	6.5	88.9	100
424 (EG)--V	40.636	0	15	8.9	75.6	100
425 (EG)--V	40.636	0	15	8.9	75.6	100
426 A2G)--V	41.172	0	4.3	0.1	95.6	100
427 (A2U)--V	41.489	0	38.8	6.2	47.3	100
428 (A2G)--V	42.223	0	2.4	4.4	93.2	100
429 (B2G)--V	43.029	0	0.1	1.5	98.5	100
430 (EU)--V	43.106	0	5.4	0.2	94.2	100
431 (EU)--V	43.106	0	5.4	0.2	94.2	100
432 (A1G)--V	43.379	0	42.3	0.7	56.9	100
433 (EU)--V	43.616	0	11.9	2.4	85	100
434 (EU)--V	43.616	0	11.9	2.4	85	100
435 (A1G)--V	44.76	0	40.6	1.6	57.3	100
436 B1G)--V	45.052	0	34.4	2.8	62.8	100
437 (B2G)--V	46.093	0	0.2	20.2	79.7	100
438 (EU)--V	46.775	0	0.8	44.4	54.2	100
439 (EU)--V	46.775	0	0.8	44.4	54.2	100

440 (A1G)--V	47.044	0	0.9	54.8	43.3	100
441 B1G)--V	47.571	0	43.7	10.5	45.7	100
442 (EU)--V	47.869	0	34.3	4	61.5	100
443 (EU)--V	47.869	0	34.3	4	61.5	100
444 (B1U)--V	47.95	0	1.5	12.5	86	100
445 (A1G)--V	48.037	0	44.4	3.3	51.8	100
446 (EG)--V	48.27	0	2.5	10.1	87.5	100
447 (EG)--V	48.27	0	2.5	10.1	87.5	100
448 (A1U)--V	48.746	0	3.6	2.7	93.7	100
449 (B1G)--V	49.193	0	53.1	1.6	45.3	100
450 (B2G)--V	49.556	0	0.1	7.9	92	100
451 (EU)--V	49.68	0	20.9	2.8	76.3	100
452 (EU)--V	49.68	0	20.9	2.8	76.3	100
453 (A1G)--V	49.803	0	18.8	4	77.1	100
454 (EU)--V	49.911	0	1.3	20.1	78.5	100
455 (EU)--V	49.911	0	1.3	20.1	78.5	100
456 A2G)--V	50.041	0	0.5	0	99.5	100
457 (A2U)--V	50.161	0	10.6	25.2	63.8	100
458 (A1G)--V	50.49	0	19.7	39.1	40.7	100
459 (EU)--V	50.95	0	6.9	1	92	100
460 (EU)--V	50.95	0	6.9	1	92	100
461 B1G)--V	50.987	0	31.1	5.2	63.7	100
462 (EG)--V	51.254	0	16	17.5	66.1	100
463 (EG)--V	51.254	0	16	17.5	66.1	100
464 (A2G)--V	51.396	0	0	0	99.9	100
465 (B2G)--V	51.664	0	0	1	98.9	100
466 (EU)--V	51.769	0	0.6	1.1	98.3	100
467 (EU)--V	51.769	0	0.6	1.1	98.3	100
468 (A1G)--V	52.02	0	10.6	37.9	51.5	100
469 (B2U)--V	52.33	0	26.1	11.5	62.4	100
470 (EU)--V	52.341	0	6.1	19.5	72.4	100
471 (EU)--V	52.341	0	6.1	19.5	72.4	100
472 (B1G)--V	52.473	0	14.5	5.5	80	100
473 (B1G)--V	52.559	0	1.5	0.3	98.2	100
474 (EU)--V	52.878	0	13.9	9.6	73.2	100
475 (EU)--V	52.878	0	13.9	9.6	73.2	100
476 (EU)--V	53.417	0	30.9	0.5	54.6	100
477 (EU)--V	53.417	0	30.9	0.5	54.6	100
478 (A2G)--V	53.77	0	0	0.7	99.3	100
479 (A1G)--V	53.828	0	7	12.3	80.1	100
480 (B2G)--V	54.309	0	0.3	8.3	91.3	100
481 B2U)--V	54.602	0	27.2	14.5	58.3	100
482 (EU)--V	54.677	0	2.8	1.1	96.1	100
483 (EU)--V	54.677	0	2.8	1.1	96.1	100
484 (EU)--V	55.464	0	7.7	4.3	87.8	100
485 (EU)--V	55.464	0	7.7	4.3	87.8	100
486 A1G)--V	55.482	0	18.4	14	67.5	100
487 (EG)--V	55.835	0	28.3	17.5	53.2	100
488 (EG)--V	55.835	0	28.3	17.5	53.2	100
489 (B1G)--V	55.907	0	28.6	4	67.4	100
490 (A2G)--V	56.884	0	7.8	4.5	87.6	100



491 B1U)--V	56.976	0	2.4	29	68.6	100
492 (EG)--V	57.057	0	5	20.1	71.8	100
493 (EG)--V	57.057	0	5	20.1	71.8	100
494 (A1U)--V	57.058	0	24.8	11.2	64.1	100
495 (A2U)--V	57.072	0	4.8	20.8	74.1	100
496 B2G)--V	57.188	0	0.2	0.2	99.6	100
497 (EU)--V	57.456	0	0.8	1.4	97.7	100
498 (EU)--V	57.456	0	0.8	1.4	97.7	100
499 (A2G)--V	57.648	0	2.3	2.4	95.3	100
500 (EU)--V	57.745	0	2.3	4.4	93.2	100
501 (EU)--V	57.745	0	2.3	4.4	93.2	100
502 (B1G)--V	58.321	0	4.6	9.1	86.3	100
503 (B2G)--V	58.437	0	0.3	6.5	93.2	100
504 (EU)--V	58.703	0	0.8	3.4	95.8	100
505 (EU)--V	58.703	0	0.8	3.4	95.8	100
506 A1G)--V	58.985	0	4.6	0.8	93.8	100
507 (EG)--V	59.23	0	14	1.4	53.6	100
508 (EG)--V	59.23	0	14	1.4	53.6	100
509 (B1U)--V	59.666	0	9.5	13.3	77.2	100
510 (EG)--V	59.925	0	8.9	3.9	38.7	100
511 (EG)--V	59.925	0	8.9	3.9	38.7	100
512 (A1U)--V	60.527	0	5.6	5	89.4	100
513 (A2G)--V	60.646	0	0	0.4	99.6	100
514 (B2U)--V	60.652	0	1	0	99	100
515 (EU)--V	60.867	0	4.1	7.2	88.7	100
516 (EU)--V	60.867	0	4.1	7.2	88.7	100
517 (EG)--V	61.217	0	9.1	0.1	90.6	100
518 (EG)--V	61.217	0	9.1	0.1	90.6	100
519 (B1U)--V	61.32	0	6.6	1.4	91.9	100
520 (EG)--V	61.508	0	1.5	6.4	89.7	100
521 (EG)--V	61.508	0	1.5	6.4	89.7	100
522 (A2U)--V	61.61	0	28	6.4	65.4	100
523 (A2U)--V	61.701	0	15.9	0.5	83.4	100
524 (A1U)--V	61.828	0	0.2	4.9	94.9	100
525 (B2G)--V	61.847	0	0.2	11.5	88.4	100
526 A2G)--V	61.942	0	3.5	1.4	95	100
527 (EU)--V	62.383	0	13.6	15.3	69	100
528 (EU)--V	62.383	0	13.6	15.3	69	100
529 (B1G)--V	62.588	0	36.3	16.6	47.1	100
530 (B2U)--V	62.736	0	2.4	1.2	96.4	100
531 (EG)--V	62.753	0	8.5	4.5	87	100
532 (EG)--V	62.753	0	8.5	4.5	87	100
533 (A1G)--V	63.487	0	1.2	17.6	81	100
534 (B2G)--V	64.253	0	4.8	5.7	83.6	100
535 (B1U)--V	64.588	0	18.2	1.8	80	100
536 (EU)--V	64.887	0	1.9	26.4	71.5	100
537 (EU)--V	64.887	0	1.9	26.4	71.5	100
538 (A2G)--V	65.539	0	0.1	0	99.9	100
539 (EG)--V	65.647	0	15.5	8.7	75.1	100
540 (EG)--V	65.647	0	15.5	8.7	75.1	100
541 (EU)--V	65.939	0	0.2	0.6	99.2	100

542 (EU)--V	65.939	0	0.2	0.6	99.2	100
543 (B2G)--V	66.161	0	2.3	24.8	72.9	100
544 (B1G)--V	66.255	0	1.8	0.1	98.1	100
545 (B2G)--V	66.879	0	4.6	5.5	89.4	100
546 A1U)--V	67.841	0	2.7	6.7	90.6	100
547 (A1G)--V	67.912	0	16.5	1.2	80.4	100
548 (A2U)--V	67.994	0	8.8	19	72	100
549 (EU)--V	68.136	0	8.8	11.6	79.5	100
550 (EU)--V	68.136	0	8.8	11.6	79.5	100
551 (EG)--V	69.075	0	7.7	10	82.4	100
552 (EG)--V	69.075	0	7.7	10	82.4	100
553 (A1U)--V	70.185	0	13.4	12.2	74.3	100
554 (B1U)--V	70.294	0	12.4	8.3	79.3	100
555 (B1G)--V	71.396	0	57.2	4.6	37.5	100
556 A1G)--V	71.402	0	18.9	35.3	43.1	100
557 (A2G)--V	71.652	0	0.6	0.2	99.1	100
558 (EU)--V	72.002	0	0.2	0.4	99.4	100
559 (EU)--V	72.002	0	0.2	0.4	99.4	100
560 (B2G)--V	72.058	0	0.3	0.1	99.6	100
561 (EG)--V	72.097	0	7	10.6	82	100
562 (EG)--V	72.097	0	7	10.6	82	100
563 (EU)--V	72.371	0	18.7	11.6	69.6	100
564 (EU)--V	72.371	0	18.7	11.6	69.6	100
565 (B1G)--V	72.598	0	0.8	2.3	97	100
566 (EU)--V	72.806	0	26.7	26.2	47	100
567 (EU)--V	72.806	0	26.7	26.2	47	100
568 (A1G)--V	72.866	0	13.1	25	60	100
569 (A2G)--V	72.934	0	3	2.1	94.8	100
570 (B1U)--V	72.936	0	0.2	4.2	95.7	100
571 (EU)--V	73.086	0	11.6	9.5	78.9	100
572 (EU)--V	73.086	0	11.6	9.5	78.9	100
573 (B1G)--V	73.228	0	27.6	4.8	67.5	100
574 (A1G)--V	73.826	0	7.8	1.8	83.6	100
575 (B2U)--V	74.094	0	15.9	30.9	53.3	100
576 A1U)--V	74.232	0	5.6	16.9	77.5	100
577 (B1G)--V	74.277	0	28.9	4.2	66.7	100
578 (EG)--V	74.29	0	10	22.4	67.3	100
579 (EG)--V	74.29	0	10	22.4	67.3	100
580 (EU)--V	74.299	0	41.9	13.6	44.4	100
581 (EU)--V	74.299	0	41.9	13.6	44.4	100
582 (A1G)--V	74.551	0	55.4	18.8	25.6	100
583 (B2G)--V	75.322	0	0.2	7.4	92.4	100
584 (B2G)--V	75.716	0	4.3	20.8	74.8	100
585 (EU)--V	76.043	0	1.7	6.2	92.1	100
586 (EU)--V	76.043	0	1.7	6.2	92.1	100
587 (A2G)--V	76.439	0	0.7	6.3	92.9	100
588 (B1G)--V	76.608	0	51.1	4.3	43.1	100
589 (B2G)--V	76.969	0	0.1	0.4	99.5	100
590 (EU)--V	77.682	0	3.1	4.6	92.3	100
591 (EU)--V	77.682	0	3.1	4.6	92.3	100
592 (EU)--V	79.149	0	7.3	4.3	88.2	100

593 (EU)--V	79.149	0	7.3	4.3	88.2	100
594 (A2G)--V	79.335	0	1.2	2.4	96.4	100
595 (A1G)--V	79.609	0	21.4	25.1	53.2	100
596 (EU)--V	79.803	0	6.2	6.6	86.8	100
597 (EU)--V	79.803	0	6.2	6.6	86.8	100
598 (B2G)--V	81.187	0	0.1	8.1	91.8	100
599 (B1G)--V	81.513	0	6.9	6.2	86	100
600 (A2G)--V	82.157	0	0.3	0.1	99.7	100
601 (EU)--V	82.839	0	10.1	10.9	78.9	100
602 (EU)--V	82.839	0	10.1	10.9	78.9	100
603 (A1G)--V	82.864	0	4.1	5.5	89.8	100
604 (A2G)--V	83.614	0	17.2	5	77.8	100
605 (B2G)--V	84.864	0	2.3	2.5	95.1	100
606 (EU)--V	85.317	0	1.1	5.6	93.3	100
607 (EU)--V	85.317	0	1.1	5.6	93.3	100
608 (EU)--V	87.741	0	7.2	19.8	72.8	100
609 (EU)--V	87.741	0	7.2	19.8	72.8	100
610 (B1G)--V	89.145	0	5.3	25.9	67.9	100
611 A1G)--V	91.039	0	4.1	55.1	40.4	100
612 (B2G)--V	91.446	0	1	1.9	97.1	100
613 (EU)--V	92.645	0	1.5	3	95.5	100
614 (EU)--V	92.645	0	1.5	3	95.5	100
615 (A2G)--V	93.357	0	6.9	12.2	80.8	100
616 A2G)--V	93.472	0	2.3	2.2	95.5	100
617 (EU)--V	95.417	0	5.6	4.5	89.8	100
618 (EU)--V	95.417	0	5.6	4.5	89.8	100
619 (B2G)--V	96.098	0	4	3.1	92.8	100

### B3PW91 Exchange Correlation Functional

Orbital	Index	E, eV	Zn	NZn	Nmeso	Pc	Total
	1 A1G)--O	-9448.41	100	0	0	0	100
	2 (A1G)--O	-1148.66	100	0	0	0	100
	3 (A2U)--O	-1012.2	100	0	0	0	100
	4 (EU)--O	-1012.02	100	0	0	0	100
	5 (EU)--O	-1012.02	100	0	0	0	100
	6 B1G)--O	-390.268	0	99.8	0	0.2	100
	7 (EU)--O	-390.268	0	99.9	0	0.1	100
	8 (EU)--O	-390.268	0	99.9	0	0.1	100
	9 (A1G)--O	-390.267	0	99.9	0	0.1	100
	10 (B2G)--O	-389.981	0	0	99.8	0.2	100
	11 (EU)--O	-389.981	0	0	99.8	0.2	100
	12 (EU)--O	-389.981	0	0	99.8	0.2	100
	13 (A1G)--O	-389.981	0	0	99.9	0.1	100
	14 (B2G)--O	-278.979	0	0	0.1	99.9	100
	15 (EU)--O	-278.979	0	0	0.1	99.9	100
	16 (EU)--O	-278.979	0	0	0.1	99.9	100
	17 (A1G)--O	-278.978	0	0	0	100	100
	18 (A2G)--O	-278.978	0	0	0	100	100

19 (EU)--O	-278.978	0	0	0	100	100
20 (EU)--O	-278.978	0	0	0	100	100
21 B1G)--O	-278.978	0	0	0	100	100
22 (EU)--O	-277.139	0	0	0	100	100
23 (EU)--O	-277.139	0	0	0	100	100
24 (A1G)--O	-277.139	0	0	0	100	100
25 (B1G)--O	-277.139	0	0	0	100	100
26 A2G)--O	-277.13	0	0	0	100	100
27 (EU)--O	-277.13	0	0	0	100	100
28 (EU)--O	-277.13	0	0	0	100	100
29 (B2G)--O	-277.13	0	0	0	100	100
30 (B1G)--O	-277.116	0	0	0	100	100
31 (EU)--O	-277.116	0	0	0	100	100
32 (EU)--O	-277.116	0	0	0	100	100
33 (A1G)--O	-277.116	0	0	0	100	100
34 (A2G)--O	-277.114	0	0	0	100	100
35 (EU)--O	-277.114	0	0	0	100	100
36 (EU)--O	-277.114	0	0	0	100	100
37 (B2G)--O	-277.114	0	0	0	100	100
38 (B1G)--O	-277.099	0	0	0	100	100
39 (EU)--O	-277.099	0	0	0	100	100
40 (EU)--O	-277.099	0	0	0	100	100
41 A1G)--O	-277.099	0	0	0	100	100
42 (A2G)--O	-277.089	0	0	0	100	100
43 (EU)--O	-277.089	0	0	0	100	100
44 (EU)--O	-277.089	0	0	0	100	100
45 (B2G)--O	-277.089	0	0	0	100	100
46 A1G)--O	-130.805	100	0	0	0	100
47 (A2U)--O	-87.163	100	0	0	0	100
48 (EU)--O	-86.882	100	0	0	0	100
49 (EU)--O	-86.882	100	0	0	0	100
50 (A1G)--O	-27.624	0.4	39.9	25.6	34.1	100
51 (EU)--O	-27.231	0.2	38.9	25.4	35.5	100
52 (EU)--O	-27.231	0.2	38.9	25.4	35.5	100
53 (B1G)--O	-26.46	0.2	59.7	0.8	39.4	100
54 (B2G)--O	-25.881	0	1.7	70.5	27.8	100
55 (EU)--O	-24.748	0	18	50.5	31.4	100
56 (EU)--O	-24.748	0	18	50.5	31.4	100
57 (A1G)--O	-23.886	0.1	16.4	49.7	33.7	100
58 (A1G)--O	-23.436	0.4	23.3	9.4	66.9	100
59 (EU)--O	-23.421	0.1	15.1	1.3	83.5	100
60 (EU)--O	-23.421	0.1	15.1	1.3	83.5	100
61 B1G)--O	-23.407	0.1	13.6	0	86.3	100
62 (A2G)--O	-21.227	0	2.7	6.5	90.8	100
63 (A1G)--O	-20.897	0.6	12.6	0.3	86.4	100
64 (EU)--O	-20.865	0.1	14.2	3.9	81.8	100
65 (EU)--O	-20.865	0.1	14.2	3.9	81.8	100
66 (EU)--O	-20.749	0	4.4	1.3	94.2	100
67 (EU)--O	-20.749	0	4.4	1.3	94.2	100
68 (B1G)--O	-20.74	0.5	19.4	0.6	79.5	100
69 (B2G)--O	-20.667	0	0	1.8	98.2	100

70 (A2G)--O	-19.756	0	5.8	9.1	85.1	100
71 (EU)--O	-19.029	0	7.4	19	73.6	100
72 (EU)--O	-19.029	0	7.4	19	73.6	100
73 (B1G)--O	-17.566	1.1	13	18.5	67.3	100
74 (A1G)--O	-17.458	2	11.7	0.3	85.9	100
75 (EU)--O	-17.282	0.2	10.9	0.3	88.6	100
76 (EU)--O	-17.282	0.2	10.9	0.3	88.6	100
77 (B2G)--O	-17.131	0.1	3.1	13.1	83.8	100
78 (B1G)--O	-16.994	0.7	4	12	83.3	100
79 (EU)--O	-16.332	0	6	3.7	90.3	100
80 (EU)--O	-16.332	0	6	3.7	90.3	100
81 B2G)--O	-16.241	2.3	31.6	22.4	43.7	100
82 (A2G)--O	-16.074	0	6.3	1.8	91.9	100
83 (A1G)--O	-15.239	3.9	9.2	1.4	85.5	100
84 (EU)--O	-15.055	0	18.7	12.7	68.6	100
85 (EU)--O	-15.055	0	18.7	12.7	68.6	100
86 B1G)--O	-14.643	13.6	14.6	5.3	66.5	100
87 (EU)--O	-14.617	0.3	15.5	19.8	64.3	100
88 (EU)--O	-14.617	0.3	15.5	19.8	64.3	100
89 (B2G)--O	-13.745	2.3	2.4	1.9	93.4	100
90 (A2G)--O	-13.728	0	27.5	15.8	56.7	100
91 B1G)--O	-13.449	50.4	14.4	0.5	34.8	100
92 (A1G)--O	-13.433	34.8	20.8	0.8	43.6	100
93 (EU)--O	-13.208	0	2.7	4.5	92.7	100
94 (EU)--O	-13.208	0	2.7	4.5	92.7	100
95 (EU)--O	-12.754	0.6	13.5	0.9	84.9	100
96 (EU)--O	-12.754	0.6	13.5	0.9	84.9	100
97 (EG)--O	-12.719	71.3	13.2	3.5	12	100
98 (EG)--O	-12.719	71.3	13.2	3.5	12	100
99 (A2U)--O	-12.708	0.4	26.2	18.4	55	100
100 (A2G)--O	-12.677	0	0.5	8.1	91.4	100
101 A1G)--O	-12.399	44.5	6.3	2.9	46.2	100
102 (B1G)--O	-12.339	17.2	7.6	1.2	74	100
103 (B2G)--O	-12.113	45.9	4.7	0.5	48.8	100
104 (A1G)--O	-12.075	17.9	1.3	3.3	77.5	100
105 (EU)--O	-12.04	0	1.2	1.5	97.2	100
106 (EU)--O	-12.04	0	1.2	1.5	97.2	100
107 (B2G)--O	-12.012	21.2	1.9	1.7	75.2	100
108 (EG)--O	-11.957	53.4	5.9	8.9	31.8	100
109 (EG)--O	-11.957	53.4	5.9	8.9	31.8	100
110 (A2G)--O	-11.742	0	0.6	4.1	95.3	100
111 (EU)--O	-11.655	0.3	5.7	4.5	89.5	100
112 (EU)--O	-11.655	0.3	5.7	4.5	89.5	100
113 (B2U)--O	-11.484	0	27.5	0	72.4	100
114 (B1G)--O	-11.334	9.5	0.9	3.9	85.7	100
115 (A1G)--O	-10.869	40.5	19.5	4.4	35.6	100
116 B1U)--O	-10.545	0	0.1	51.7	48.3	100
117 (B2G)--O	-10.162	0.4	0.1	1.8	97.7	100
118 (EU)--O	-10.081	0.1	2	2.6	95.3	100
119 (EU)--O	-10.081	0.1	2	2.6	95.3	100
120 (EG)--O	-10.001	0.9	2.7	13.9	82.5	100

121 (EG)--O	-10.001	0.9	2.7	13.9	82.5	100
122 (A2U)--O	-9.978	0.3	7.6	3.8	88.4	100
123 (A2G)--O	-9.867	0	2	1.2	96.9	100
124 (EU)--O	-9.744	4.1	36	3.1	56.7	100
125 (EU)--O	-9.744	4.1	36	3.1	56.7	100
126 A1G)--O	-9.697	0	1.8	3.2	95	100
127 (B2U)--O	-9.557	0	27.3	0	72.7	100
128 (B1G)--O	-9.337	1.4	1.1	2.9	94.6	100
129 (EU)--O	-9.331	1.9	15	6.8	76.3	100
130 (EU)--O	-9.331	1.9	15	6.8	76.3	100
131 (EG)--O	-8.785	1.7	22	21.9	54.3	100
132 (EG)--O	-8.785	1.7	22	21.9	54.3	100
133 (A1G)--O	-8.373	0.3	17.6	55.4	26.8	100
134 (A1U)--O	-7.642	0	0	0	99.9	100
135 (EU)--O	-7.617	0.2	18.4	51.1	30.2	100
136 (EU)--O	-7.617	0.2	18.4	51.1	30.2	100
137 (A2U)--O	-7.191	2.5	46.5	19.8	31.2	100
138 (B2G)--O	-7.12	0.6	12.8	62.6	24.1	100
139 (B1U)--O	-7.113	0	0	5.2	94.8	100
140 (EG)--O	-7.083	0	0.6	10	89.4	100
141 (EG)--O	-7.083	0	0.6	10	89.4	100
142 (A2U)--O	-6.919	0.2	6.6	40.2	53	100
143 (EG)--O	-6.887	1.3	27.8	1.3	69.6	100
144 (EG)--O	-6.887	1.3	27.8	1.3	69.6	100
145 (B2U)--O	-6.857	0	25.2	0	74.8	100
146 B1G)--O	-6.745	20.5	53.5	0.9	25.1	100
147 (A1U)--O	-5.073	0	0.1	0.1	99.8	100
148 (EG)--V	-2.88	0.3	13.3	19	67.4	100
149 (EG)--V	-2.88	0.3	13.3	19	67.4	100
150 (B1U)--V	-1.192	0	0	23.7	76.3	100
151 B2U)--V	-0.941	0	19	0	80.9	100
152 (A2U)--V	-0.778	6	1.1	5.5	87.4	100
153 (EG)--V	-0.635	0.1	5.3	3.6	91.1	100
154 (EG)--V	-0.635	0.1	5.3	3.6	91.1	100
155 (A1U)--V	0.636	0	0	0	100	100
156 (EG)--V	0.711	0	1.8	1	97.2	100
157 (EG)--V	0.711	0	1.8	1	97.2	100
158 (A2U)--V	0.935	63.7	7.1	2.2	27	100
159 (A1G)--V	1.18	73.5	15.7	0.3	10.6	100
160 (B2U)--V	1.347	0	19.4	0.1	80.5	100
161 B1U)--V	1.596	0	0.1	19.2	80.8	100
162 (A1G)--V	2.767	0.3	0.1	1.7	97.9	100
163 (EU)--V	2.794	22.2	2.9	1.6	73.2	100
164 (EU)--V	2.794	22.2	2.9	1.6	73.2	100
165 (B1G)--V	2.965	0	0	0.1	99.9	100
166 (EG)--V	3.018	0.1	14.3	16	69.6	100
167 (EG)--V	3.018	0.1	14.3	16	69.6	100
168 (EU)--V	3.023	46.5	5.2	1	47.3	100
169 (EU)--V	3.023	46.5	5.2	1	47.3	100
170 (A2U)--V	3.648	33.1	14.7	15.6	36.5	100
171 B2G)--V	3.825	0	1	0.2	98.8	100

172 (EU)--V	4.028	0	1.1	0.2	98.7	100
173 (EU)--V	4.028	0	1.1	0.2	98.7	100
174 (A1G)--V	4.115	29.4	0.4	10.5	59.7	100
175 (A2G)--V	4.277	0	0.7	0	99.3	100
176 (EU)--V	4.709	1.1	0.1	3.3	95.5	100
177 (EU)--V	4.709	1.1	0.1	3.3	95.5	100
178 (B2G)--V	4.73	0	0.1	4.9	95	100
179 (A1U)--V	4.766	0	0	0	100	100
180 (EG)--V	4.955	0	0.9	4.1	95	100
181 (EG)--V	4.955	0	0.9	4.1	95	100
182 (B1U)--V	4.966	0	0	4.6	95.4	100
183 (A1G)--V	5.035	33	1	0.3	65.7	100
184 (EU)--V	5.109	0.9	2	0.2	96.9	100
185 (EU)--V	5.109	0.9	2	0.2	96.9	100
186 B1G)--V	5.119	0	4.7	0.2	95.1	100
187 (A2G)--V	5.293	0	0.1	0	99.9	100
188 (EU)--V	5.839	5.3	9.2	4.2	81.3	100
189 (EU)--V	5.839	5.3	9.2	4.2	81.3	100
190 (B2G)--V	5.846	0.1	3	11.2	85.7	100
191 A1G)--V	6.09	0	0.7	1.3	98	100
192 (B1G)--V	6.144	0	28.6	3.5	67.9	100
193 (A2U)--V	6.618	84.9	3.9	1.7	9.5	100
194 (EU)--V	6.628	0.2	0.7	1.8	97.3	100
195 (EU)--V	6.628	0.2	0.7	1.8	97.3	100
196 A2G)--V	6.77	0	5.7	0.6	93.7	100
197 (B2G)--V	6.992	0	0.3	11.5	88.2	100
198 (EU)--V	7.002	0.8	0.2	5.6	93.4	100
199 (EU)--V	7.002	0.8	0.2	5.6	93.4	100
200 (A2G)--V	7.291	0	0.2	0	99.8	100
201 B1G)--V	7.313	0	2	0	98	100
202 (A1G)--V	7.671	7.7	9.5	21.2	61.5	100
203 (EU)--V	7.683	1.3	4.4	1.9	92.4	100
204 (EU)--V	7.683	1.3	4.4	1.9	92.4	100
205 (EU)--V	8.086	0.9	8.1	3	88	100
206 (EU)--V	8.086	0.9	8.1	3	88	100
207 (A1G)--V	8.169	5.4	0.6	3	91	100
208 (B1G)--V	8.795	0	0.3	0.1	99.6	100
209 (B2G)--V	8.802	0	0.8	3.7	95.5	100
210 (EU)--V	9.119	0.4	2.2	13.4	84	100
211 (EU)--V	9.119	0.4	2.2	13.4	84	100
212 (A1G)--V	9.341	0.3	1.9	2.3	95.5	100
213 (EU)--V	9.383	1.6	5	1.7	91.8	100
214 (EU)--V	9.383	1.6	5	1.7	91.8	100
215 (B2G)--V	9.699	0	4.3	24.5	71.2	100
216 B1G)--V	9.934	0	4.1	0.1	95.8	100
217 (B2G)--V	10.221	0	1.2	12.9	85.9	100
218 (EU)--V	10.611	2.4	3.7	17.4	76.5	100
219 (EU)--V	10.611	2.4	3.7	17.4	76.5	100
220 (A1G)--V	10.677	1.1	17	12.8	69.1	100
221 A2G)--V	10.695	0	6.9	8.4	84.6	100
222 (A2G)--V	11.514	0	0	0.8	99.2	100

223 (EU)--V	11.546	2.8	11.2	8.2	77.9	100
224 (EU)--V	11.546	2.8	11.2	8.2	77.9	100
225 (B1G)--V	11.682	0	19.4	8.1	72.4	100
226 (EU)--V	11.683	0.7	1.3	3.5	94.5	100
227 (EU)--V	11.683	0.7	1.3	3.5	94.5	100
228 (EU)--V	13.482	2	3.8	3.6	90.5	100
229 (EU)--V	13.482	2	3.8	3.6	90.5	100
230 (A2G)--V	13.68	0	0.2	6.2	93.5	100
231 B2G)--V	13.883	0	0.3	0	99.6	100
232 (EG)--V	13.939	0	1.4	1.3	97.2	100
233 (EG)--V	13.939	0	1.4	1.3	97.2	100
234 (B2U)--V	14.152	0	0.4	0	99.6	100
235 (A2U)--V	14.257	3.7	0.2	0.7	95.5	100
236 (EU)--V	14.655	0.2	0.5	2.7	96.6	100
237 (EU)--V	14.655	0.2	0.5	2.7	96.6	100
238 (A1G)--V	14.761	0.7	3.8	0.8	94.7	100
239 (EG)--V	14.809	0	2.1	1.6	96.3	100
240 (EG)--V	14.809	0	2.1	1.6	96.3	100
241 B1G)--V	14.944	0	34.1	5	60.9	100
242 (A2G)--V	14.984	0	0.9	2.7	96.4	100
243 (B1U)--V	15.106	0	0	4.3	95.7	100
244 (B2G)--V	15.235	0	0.3	1.3	98.4	100
245 (EU)--V	15.246	0.2	0.4	0.3	99.1	100
246 (EU)--V	15.246	0.2	0.4	0.3	99.1	100
247 (B1G)--V	15.435	0	4.9	2	93	100
248 (EU)--V	15.483	0	0.5	1.2	98.3	100
249 (EU)--V	15.483	0	0.5	1.2	98.3	100
250 (B2U)--V	15.634	0	1.3	0.1	98.6	100
251 B2G)--V	15.66	0	0.9	1.7	97.5	100
252 (A2U)--V	15.731	9.6	1.4	1.4	87.6	100
253 (A2G)--V	15.747	0	0.3	0.9	98.9	100
254 (A1G)--V	15.773	1.7	1.3	12.8	84.2	100
255 (EG)--V	15.929	0	0.5	1.6	97.9	100
256 (EG)--V	15.929	0	0.5	1.6	97.9	100
257 (EU)--V	15.96	0.1	1	1.2	97.7	100
258 (EU)--V	15.96	0.1	1	1.2	97.7	100
259 (B1G)--V	16.056	0	25.1	1.1	73.9	100
260 (A1U)--V	16.068	0	0	0	100	100
261 A1G)--V	16.554	1.2	0.4	9.9	88.5	100
262 (EU)--V	16.56	0.3	16.3	14.9	68.5	100
263 (EU)--V	16.56	0.3	16.3	14.9	68.5	100
264 (A2G)--V	16.734	0	0.9	1.4	97.7	100
265 (B1G)--V	16.772	0	0.4	1	98.6	100
266 (EU)--V	16.78	0.2	0.9	0.5	98.5	100
267 (EU)--V	16.78	0.2	0.9	0.5	98.5	100
268 (A1G)--V	16.822	0.9	23	8	68.1	100
269 (B2G)--V	16.828	0	0.7	8.6	90.7	100
270 (B1U)--V	16.882	0	0	1.1	98.9	100
271 (EG)--V	17.102	0	3.7	0.6	95.7	100
272 (EG)--V	17.102	0	3.7	0.6	95.7	100
273 (A1G)--V	17.108	0.4	14.7	22.2	62.6	100



274 (EU)--V	17.133	1.3	23.2	9.9	65.6	100
275 (EU)--V	17.133	1.3	23.2	9.9	65.6	100
276 A2G)--V	17.408	0	1	3.2	95.9	100
277 (EU)--V	17.732	1.9	3.5	1.4	93.1	100
278 (EU)--V	17.732	1.9	3.5	1.4	93.1	100
279 (EG)--V	17.821	0	1.2	3.5	95.4	100
280 (EG)--V	17.821	0	1.2	3.5	95.4	100
281 A2U)--V	17.841	2.9	1.1	1.2	94.8	100
282 (EU)--V	17.877	1	1.5	14.2	83.2	100
283 (EU)--V	17.877	1	1.5	14.2	83.2	100
284 (B2G)--V	17.949	0	0.6	14	85.4	100
285 (B2U)--V	17.962	0	1.7	0	98.3	100
286 A1U)--V	18.021	0	0	0	100	100
287 (B1G)--V	18.363	0.1	12.2	9	78.8	100
288 (B1U)--V	18.718	0	0	2.3	97.7	100
289 (EG)--V	18.836	0	0.6	0.3	99.2	100
290 (EG)--V	18.836	0	0.6	0.3	99.2	100
291 A2U)--V	19.021	0.6	0.4	3.6	95.4	100
292 (A1G)--V	19.215	5.9	22.2	4.1	67.8	100
293 (B2U)--V	20.272	0	1	0	99	100
294 (EG)--V	20.337	0	1.3	1.7	97.1	100
295 (EG)--V	20.337	0	1.3	1.7	97.1	100
296 A1U)--V	20.538	0	0	0	100	100
297 (EU)--V	20.608	5.5	14.9	7.2	72.3	100
298 (EU)--V	20.608	5.5	14.9	7.2	72.3	100
299 (B1U)--V	21.074	0	0	3.4	96.6	100
300 (EG)--V	21.574	0.2	34.5	6.4	58.9	100
301 (EG)--V	21.574	0.2	34.5	6.4	58.9	100
302 (B2G)--V	21.801	0	0.2	3.3	96.5	100
303 (EU)--V	22.01	0.1	1.2	1.7	97	100
304 (EU)--V	22.01	0.1	1.2	1.7	97	100
305 (A1G)--V	22.139	0.1	0.4	1	98.5	100
306 A2U)--V	22.398	1.2	12	56.9	29.9	100
307 (B2G)--V	22.484	0	2	1.5	96.4	100
308 (EG)--V	22.687	0	2.5	0.5	97	100
309 (EG)--V	22.687	0	2.5	0.5	97	100
310 (A2G)--V	22.712	0	0.3	1.1	98.6	100
311 (EU)--V	22.779	0.1	0	1.1	98.8	100
312 (EU)--V	22.779	0.1	0	1.1	98.8	100
313 (A2G)--V	23.081	0	1.7	0.9	97.4	100
314 (EU)--V	23.219	0	0.9	0.3	98.8	100
315 (EU)--V	23.219	0	0.9	0.3	98.8	100
316 B1G)--V	23.26	0	1.1	0.6	98.3	100
317 (B2G)--V	23.452	0	7.3	10.9	81.9	100
318 (A1G)--V	23.665	0.5	9.7	7.5	82.4	100
319 (B2G)--V	23.677	0	5	1.3	93.7	100
320 (EU)--V	23.78	0.2	2.1	3.8	94	100
321 (EU)--V	23.78	0.2	2.1	3.8	94	100
322 (B2U)--V	24.182	0	69	0	31	100
323 (A2G)--V	24.187	0	0.5	8.6	90.9	100
324 (A1U)--V	24.25	0	0	0	100	100

325 (B1G)--V	24.382	0	0.5	0	99.5	100
326 (EU)--V	24.383	0.1	0.8	3.3	95.7	100
327 (EU)--V	24.383	0.1	0.8	3.3	95.7	100
328 (A1G)--V	24.499	2.4	2.5	25.8	69.3	100
329 (EG)--V	24.932	0.1	14.3	41.9	43.7	100
330 (EG)--V	24.932	0.1	14.3	41.9	43.7	100
331 B1U)--V	25.009	0	0	63.9	36.1	100
332 (B1G)--V	25.042	0	20.2	11	68.8	100
333 (A1G)--V	25.222	0.8	10	6.1	83.1	100
334 (EU)--V	25.307	0.3	3.3	7.1	89.3	100
335 (EU)--V	25.307	0.3	3.3	7.1	89.3	100
336 (EU)--V	25.665	0.4	9.8	5.3	84.6	100
337 (EU)--V	25.665	0.4	9.8	5.3	84.6	100
338 (A2G)--V	25.816	0	0	0	100	100
339 (B1G)--V	25.964	0	0.3	0.3	99.4	100
340 (EU)--V	26.332	0.4	0.2	4.2	95.2	100
341 (EU)--V	26.332	0.4	0.2	4.2	95.2	100
342 (B2G)--V	26.903	0	0.1	0.8	99	100
343 (A2U)--V	27.004	4.6	43.4	15.9	36.1	100
344 (A2G)--V	27.096	0	0	1.7	98.3	100
345 (EU)--V	27.127	0.1	1.2	2.6	96.1	100
346 (EU)--V	27.127	0.1	1.2	2.6	96.1	100
347 (B2G)--V	27.439	0	1	1.9	97.1	100
348 (B1G)--V	27.574	0	7.9	2.1	90	100
349 (EU)--V	27.762	0.4	6.1	3.3	90.1	100
350 (EU)--V	27.762	0.4	6.1	3.3	90.1	100
351 (EU)--V	28.183	0	5.7	5.7	88.6	100
352 (EU)--V	28.183	0	5.7	5.7	88.6	100
353 (A1G)--V	28.212	0	3.3	3.4	93.3	100
354 (A1G)--V	28.464	0.2	5.7	6.5	87.6	100
355 (B2G)--V	28.957	0	7.2	4	88.9	100
356 (EU)--V	29.401	0	2.3	2.9	94.7	100
357 (EU)--V	29.401	0	2.3	2.9	94.7	100
358 (A2G)--V	29.461	0	0.8	0.2	99.1	100
359 (A2G)--V	30.456	0	2.9	2.4	94.7	100
360 (B1G)--V	30.621	0	0.9	15	84.1	100
361 (EU)--V	30.706	0.1	1	0.8	98.2	100
362 (EU)--V	30.706	0.1	1	0.8	98.2	100
363 (B2G)--V	30.862	0	0.9	4.2	94.9	100
364 (B1G)--V	31.105	0	4.9	12.2	82.9	100
365 (A1G)--V	31.412	0.8	6.2	3.7	89.3	100
366 (EU)--V	31.525	0.1	5.6	3.3	91	100
367 (EU)--V	31.525	0.1	5.6	3.3	91	100
368 (B2G)--V	31.86	0	1.6	3.1	95.2	100
369 (A1G)--V	32.621	5.3	3.6	0.4	90.7	100
370 (B2U)--V	32.631	0	7.9	8.3	83.7	100
371 (EU)--V	32.824	1	6.3	4.7	88	100
372 (EU)--V	32.824	1	6.3	4.7	88	100
373 (EG)--V	33.031	0.1	5.4	14.4	80	100
374 (EG)--V	33.031	0.1	5.4	14.4	80	100
375 (A2G)--V	33.045	0	1.1	14.3	84.6	100

376 A2U)--V	33.662	0.2	0.9	10.9	88	100
377 (B1G)--V	33.76	0.3	13	8.8	77.9	100
378 (EU)--V	33.949	0.2	3.5	9.5	86.7	100
379 (EU)--V	33.949	0.2	3.5	9.5	86.7	100
380 (B2G)--V	34.228	0	1.7	1.9	96.4	100
381 A1U)--V	34.569	0	19.8	18.1	62.2	100
382 (EG)--V	34.601	0	8.7	9.7	81.5	100
383 (EG)--V	34.601	0	8.7	9.7	81.5	100
384 (B2U)--V	34.689	0	6.5	9.7	83.8	100
385 (EU)--V	34.988	0.2	1.7	12.5	85.7	100
386 (EU)--V	34.988	0.2	1.7	12.5	85.7	100
387 (A2G)--V	35.42	0	0.8	8.6	90.6	100
388 (B1U)--V	35.606	0	5.2	6.8	88	100
389 (EG)--V	35.699	0.2	5.2	7.3	87.4	100
390 (EG)--V	35.699	0.2	5.2	7.3	87.4	100
391 B1G)--V	35.831	0	0.4	4.3	95.2	100
392 (A1U)--V	35.934	0	3.6	5.7	90.7	100
393 (A2U)--V	36.445	4.2	27.4	17.2	51.1	100
394 (EG)--V	36.587	1.9	18.6	7.9	71.6	100
395 (EG)--V	36.587	1.9	18.6	7.9	71.6	100
396 A1G)--V	36.693	3.5	5.8	0.1	90.6	100
397 (EU)--V	36.762	0.1	3.8	0.6	95.5	100
398 (EU)--V	36.762	0.1	3.8	0.6	95.5	100
399 (B1G)--V	36.769	0	6	0.2	93.8	100
400 (EU)--V	37.569	0.3	6.7	0.2	92.8	100
401 (EU)--V	37.569	0.3	6.7	0.2	92.8	100
402 (B2U)--V	38.232	0	28.1	0.7	71.2	100
403 (A1G)--V	38.622	0.1	0.4	0	99.5	100
404 (A2G)--V	38.85	0	3	17.5	79.5	100
405 (B2G)--V	38.854	0	0.1	0.4	99.5	100
406 (EU)--V	38.874	0.1	1.1	1.6	97.2	100
407 (EU)--V	38.874	0.1	1.1	1.6	97.2	100
408 (B1G)--V	38.943	0	0.1	1.2	98.7	100
409 (EG)--V	39.031	0.1	3.8	5.8	90.2	100
410 (EG)--V	39.031	0.1	3.8	5.8	90.2	100
411 A2U)--V	39.047	0.5	1.9	2	95.5	100
412 (B2U)--V	39.118	0	0.2	0.7	99.2	100
413 (EG)--V	39.381	0.4	12.4	11.9	75.2	100
414 (EG)--V	39.381	0.4	12.4	11.9	75.2	100
415 (A2U)--V	39.608	2.4	10.2	0.7	86.7	100
416 B2U)--V	39.969	0	2.2	0.7	97	100
417 (B1U)--V	39.972	0	18.3	23.7	57.9	100
418 (EG)--V	40.244	0.2	5.6	2.8	91.4	100
419 (EG)--V	40.244	0.2	5.6	2.8	91.4	100
420 (A1U)--V	40.28	0	0	0	100	100
421 B1U)--V	40.342	0	4.1	5.7	90.2	100
422 (EG)--V	40.371	0.6	14.4	8.6	76.5	100
423 (EG)--V	40.371	0.6	14.4	8.6	76.5	100
424 (EU)--V	40.525	0	1.4	0.8	97.9	100
425 (EU)--V	40.525	0	1.4	0.8	97.9	100
426 A2G)--V	41.139	0	4.3	0	95.6	100

427 (A2U)--V	41.229	7.9	38.8	6.1	47.2	100
428 (A2G)--V	42.196	0	2.3	4.4	93.3	100
429 (B2G)--V	42.939	0	0.1	1.5	98.4	100
430 (EU)--V	42.984	0.2	4.7	0.2	94.9	100
431 (EU)--V	42.984	0.2	4.7	0.2	94.9	100
432 (A1G)--V	43.252	0.1	41.9	0.7	57.4	100
433 (EU)--V	43.516	0.7	13.2	2.6	83.5	100
434 (EU)--V	43.516	0.7	13.2	2.6	83.5	100
435 (A1G)--V	44.558	0.5	41.3	1.4	56.8	100
436 B1G)--V	44.917	0	33.7	2.7	63.6	100
437 (B2G)--V	45.97	0	0.2	19.7	80.1	100
438 (EU)--V	46.609	0.7	0.9	43.9	54.4	100
439 (EU)--V	46.609	0.7	0.9	43.9	54.4	100
440 (A1G)--V	46.903	1.1	0.9	54.1	44	100
441 B1G)--V	47.427	0	43.6	10.6	45.8	100
442 (EU)--V	47.729	0.2	34.9	4.1	60.8	100
443 (EU)--V	47.729	0.2	34.9	4.1	60.8	100
444 (B1U)--V	47.737	0	1.5	12.5	86.1	100
445 (A1G)--V	47.897	0.6	44.4	3.4	51.6	100
446 (EG)--V	48.057	0	2.4	10	87.5	100
447 (EG)--V	48.057	0	2.4	10	87.5	100
448 (A1U)--V	48.528	0	3.6	2.7	93.8	100
449 (B1G)--V	49.026	0	53.3	1.3	45.4	100
450 (B2G)--V	49.466	0	0.1	8.8	91.1	100
451 (EU)--V	49.54	0.1	21.5	2.6	75.8	100
452 (EU)--V	49.54	0.1	21.5	2.6	75.8	100
453 (A1G)--V	49.609	0.1	17.3	6.3	76.3	100
454 (EU)--V	49.785	0.1	0.9	21.6	77.3	100
455 (EU)--V	49.785	0.1	0.9	21.6	77.3	100
456 A2U)--V	49.934	0.5	10.6	25.2	63.8	100
457 (A2G)--V	50.019	0	0.5	0	99.5	100
458 (A1G)--V	50.36	0.6	19.9	38.6	40.9	100
459 (EU)--V	50.833	0	8	1.1	90.8	100
460 (EU)--V	50.833	0	8	1.1	90.8	100
461 B1G)--V	50.86	0	31.2	5.1	63.7	100
462 (EG)--V	51.024	0.4	15.8	17.5	66.2	100
463 (EG)--V	51.024	0.4	15.8	17.5	66.2	100
464 (A2G)--V	51.311	0	0	0	99.9	100
465 (B2G)--V	51.675	0	0	1	98.9	100
466 (EU)--V	51.767	0	0.5	1.1	98.4	100
467 (EU)--V	51.767	0	0.5	1.1	98.4	100
468 (A1G)--V	51.904	0	10.8	37.7	51.6	100
469 (B2U)--V	52.096	0	26	11.4	62.6	100
470 (EU)--V	52.235	1.7	5.7	18.1	74.4	100
471 (EU)--V	52.235	1.7	5.7	18.1	74.4	100
472 (B1G)--V	52.326	0	14.8	5.6	79.6	100
473 (B1G)--V	52.451	0	1.1	0.1	98.7	100
474 (EU)--V	52.756	2.6	13.5	9.5	74.5	100
475 (EU)--V	52.756	2.6	13.5	9.5	74.5	100
476 (EU)--V	53.353	15.1	31.8	0.5	52.6	100
477 (EU)--V	53.353	15.1	31.8	0.5	52.6	100

478 (A1G)--V	53.665	0.6	7.2	12.1	80.2	100
479 (A2G)--V	53.68	0	0	0.6	99.3	100
480 (B2G)--V	54.169	0	0.3	8.2	91.4	100
481 (B2U)--V	54.345	0	27.3	14.5	58.1	100
482 (EU)--V	54.547	0	2.8	1.1	96.2	100
483 (EU)--V	54.547	0	2.8	1.1	96.2	100
484 (EU)--V	55.318	0.1	7.8	4.3	87.8	100
485 (EU)--V	55.318	0.1	7.8	4.3	87.8	100
486 (A1G)--V	55.355	0	18.4	14	67.5	100
487 (EG)--V	55.587	0.9	28.4	17.6	53.1	100
488 (EG)--V	55.587	0.9	28.4	17.6	53.1	100
489 (B1G)--V	55.767	0	28.7	4.1	67.1	100
490 (B1U)--V	56.731	0	2.4	29.1	68.5	100
491 (A2G)--V	56.758	0	8.2	4.7	87.1	100
492 (A1U)--V	56.808	0	24.8	11.1	64.1	100
493 (EG)--V	56.822	2.5	5.1	20.2	72.2	100
494 (EG)--V	56.822	2.5	5.1	20.2	72.2	100
495 (A2U)--V	56.832	0.3	4.8	20.8	74	100
496 (B2G)--V	57.038	0	0.2	0.2	99.7	100
497 (EU)--V	57.321	0.1	0.8	1.6	97.5	100
498 (EU)--V	57.321	0.1	0.8	1.6	97.5	100
499 (A2G)--V	57.571	0	2.4	2.4	95.2	100
500 (EU)--V	57.609	0	2.2	4.1	93.7	100
501 (EU)--V	57.609	0	2.2	4.1	93.7	100
502 (B1G)--V	58.163	0	4.6	9.1	86.3	100
503 (B2G)--V	58.302	0	0.3	6.4	93.2	100
504 (EU)--V	58.555	0.1	0.8	3.4	95.7	100
505 (EU)--V	58.555	0.1	0.8	3.4	95.7	100
506 (A1G)--V	58.831	0.8	4.6	0.8	93.8	100
507 (EG)--V	59.071	17.8	13.8	2.1	66.2	100
508 (EG)--V	59.071	17.8	13.8	2.1	66.2	100
509 (B1U)--V	59.398	0	9.8	13.2	77	100
510 (EG)--V	59.878	61.6	9.3	2.8	26.3	100
511 (EG)--V	59.878	61.6	9.3	2.8	26.3	100
512 (A1U)--V	60.288	0	5.6	5	89.4	100
513 (B2U)--V	60.401	0	1	0	99	100
514 (A2G)--V	60.494	0	0	0.4	99.5	100
515 (EU)--V	60.72	0	4.2	7.4	88.4	100
516 (EU)--V	60.72	0	4.2	7.4	88.4	100
517 (EG)--V	60.971	0.4	8.9	0.1	90.6	100
518 (EG)--V	60.971	0.4	8.9	0.1	90.6	100
519 (B1U)--V	61.082	0	6.5	1.5	92	100
520 (EG)--V	61.273	3.4	1.8	6.4	88.4	100
521 (EG)--V	61.273	3.4	1.8	6.4	88.4	100
522 (A2U)--V	61.349	0.3	31.4	6	62.3	100
523 (A2U)--V	61.442	0.1	11.7	0.9	87.3	100
524 (A1U)--V	61.569	0	0.2	4.9	94.9	100
525 (B2G)--V	61.703	0	0.2	11.6	88.2	100
526 (A2G)--V	61.78	0	3.5	1.4	95.1	100
527 (EU)--V	62.219	2.2	13.5	15.1	69.2	100
528 (EU)--V	62.219	2.2	13.5	15.1	69.2	100

529 (B1G)--V	62.449	0	36	16.6	47.4	100
530 (B2U)--V	62.47	0	2.4	1.2	96.4	100
531 (EG)--V	62.493	0	8.5	4.6	87	100
532 (EG)--V	62.493	0	8.5	4.6	87	100
533 (A1G)--V	63.327	0.1	1.2	17.6	81	100
534 (B2G)--V	64.244	5.6	3.9	8.2	82.2	100
535 (B1U)--V	64.324	0	18.2	1.7	80.1	100
536 (EU)--V	64.746	0.1	1.9	26.5	71.5	100
537 (EU)--V	64.746	0.1	1.9	26.5	71.5	100
538 (EG)--V	65.38	0.8	15.5	8.6	75	100
539 (EG)--V	65.38	0.8	15.5	8.6	75	100
540 (A2G)--V	65.424	0	0.1	0	99.9	100
541 (EU)--V	65.812	0	0.2	0.6	99.1	100
542 (EU)--V	65.812	0	0.2	0.6	99.1	100
543 (B2G)--V	66.065	0	2.2	24.2	73.6	100
544 (B1G)--V	66.109	0	1.8	0	98.1	100
545 (B2G)--V	66.782	0.7	5.4	7.7	86.3	100
546 A1U)--V	67.578	0	2.6	6.7	90.6	100
547 (A2U)--V	67.732	0.2	8.8	19	72	100
548 (A1G)--V	67.789	1.9	16.2	1.1	80.9	100
549 (EU)--V	67.99	0.2	8.8	11.6	79.4	100
550 (EU)--V	67.99	0.2	8.8	11.6	79.4	100
551 (EG)--V	68.811	0	7.6	10	82.4	100
552 (EG)--V	68.811	0	7.6	10	82.4	100
553 (A1U)--V	69.908	0	13.5	12.3	74.2	100
554 (B1U)--V	70.029	0	12.3	8.3	79.3	100
555 (A1G)--V	71.312	2.5	19.3	35.3	42.8	100
556 B1G)--V	71.323	0.6	56.7	4.7	37.9	100
557 (A2G)--V	71.519	0	0.6	0.2	99.2	100
558 (EG)--V	71.834	0.4	7.1	10.7	81.9	100
559 (EG)--V	71.834	0.4	7.1	10.7	81.9	100
560 (EU)--V	71.858	0	0.2	0.4	99.4	100
561 (EU)--V	71.858	0	0.2	0.4	99.4	100
562 (B2G)--V	71.914	0	0.3	0.1	99.6	100
563 (EU)--V	72.265	0.1	19.5	12.3	68.1	100
564 (EU)--V	72.265	0.1	19.5	12.3	68.1	100
565 (B1G)--V	72.492	0	0.5	2.2	97.3	100
566 (EU)--V	72.676	0.1	25.6	26.6	47.7	100
567 (EU)--V	72.676	0.1	25.6	26.6	47.7	100
568 (B1U)--V	72.676	0	0.2	4.2	95.7	100
569 (A1G)--V	72.762	1.6	13	24.6	60.9	100
570 (A2G)--V	72.786	0	3	2.2	94.9	100
571 (EU)--V	72.947	0	11.8	9.7	78.4	100
572 (EU)--V	72.947	0	11.8	9.7	78.4	100
573 (B1G)--V	73.071	0	28.5	4.6	66.9	100
574 (A1G)--V	73.797	6.9	10.2	4	78.9	100
575 (B2U)--V	73.817	0	15.9	30.8	53.3	100
576 A1U)--V	73.961	0	5.5	16.8	77.7	100
577 (EG)--V	74.018	0.2	10	22.3	67.5	100
578 (EG)--V	74.018	0.2	10	22.3	67.5	100
579 (EU)--V	74.181	0.1	42.4	13.7	43.8	100

580 (EU)--V	74.181	0.1	42.4	13.7	43.8	100
581 B1G)--V	74.187	0.2	30.2	4.4	65.2	100
582 (A1G)--V	74.449	0.4	55.5	18.3	25.8	100
583 (B2G)--V	75.212	0	0.2	7.4	92.3	100
584 (B2G)--V	75.606	0.1	4.3	20.3	75.3	100
585 (EU)--V	75.939	0	1.7	6.2	92.1	100
586 (EU)--V	75.939	0	1.7	6.2	92.1	100
587 (A2G)--V	76.342	0	0.7	6.2	93	100
588 (B1G)--V	76.537	1.5	50	4.1	44.4	100
589 (B2G)--V	76.849	0	0.1	0.5	99.4	100
590 (EU)--V	77.569	0	3.1	4.7	92.2	100
591 (EU)--V	77.569	0	3.1	4.7	92.2	100
592 (EU)--V	79.012	0.1	7.4	4.4	88.1	100
593 (EU)--V	79.012	0.1	7.4	4.4	88.1	100
594 (A2G)--V	79.239	0	1.2	2.4	96.4	100
595 (A1G)--V	79.461	0.3	21.4	25.2	53.1	100
596 (EU)--V	79.64	0.4	6.1	6.5	87.1	100
597 (EU)--V	79.64	0.4	6.1	6.5	87.1	100
598 (B2G)--V	81.068	0	0.1	8.1	91.7	100
599 (B1G)--V	81.419	0.9	7.1	6.3	85.7	100
600 (A2G)--V	82.036	0	0.3	0.1	99.7	100
601 A1G)--V	82.701	0.6	4.1	5.1	90.2	100
602 (EU)--V	82.727	0.1	10.1	10.8	79	100
603 (EU)--V	82.727	0.1	10.1	10.8	79	100
604 (A2G)--V	83.527	0	17.3	5.1	77.6	100
605 (B2G)--V	84.723	0	2.4	2.6	95.1	100
606 (EU)--V	85.169	0	1.1	5.6	93.2	100
607 (EU)--V	85.169	0	1.1	5.6	93.2	100
608 (EU)--V	87.577	0.2	7.2	19.8	72.9	100
609 (EU)--V	87.577	0.2	7.2	19.8	72.9	100
610 (B1G)--V	89.004	0.9	5.3	26	67.7	100
611 A1G)--V	90.854	0.4	4	55.3	40.3	100
612 (B2G)--V	91.287	0	1	1.8	97.2	100
613 (EU)--V	92.487	0	1.5	3	95.5	100
614 (EU)--V	92.487	0	1.5	3	95.5	100
615 (A2G)--V	93.211	0	6	11.1	82.9	100
616 A2G)--V	93.329	0	3	3.1	93.9	100
617 (EU)--V	95.263	0	5.6	4.5	89.9	100
618 (EU)--V	95.263	0	5.6	4.5	89.9	100
619 (B2G)--V	95.945	0	4	3.1	92.9	100

### B3P86 Exchange Correlation Functional

Orbital	Index	E, eV	Zn	NZn	Nmeso	Pc	Total
	1 A1G)--O	-9449.7	100	0	0	0	100
	2 (A1G)--O	-1149.38	100	0	0	0	100
	3 (A2U)--O	-1012.76	100	0	0	0	100
	4 (EU)--O	-1012.57	100	0	0	0	100
	5 (EU)--O	-1012.57	100	0	0	0	100

6 B1G)--O	-390.869	0	99.8	0	0.2	100
7 (EU)--O	-390.869	0	99.9	0	0.1	100
8 (EU)--O	-390.869	0	99.9	0	0.1	100
9 (A1G)--O	-390.868	0	99.9	0	0.1	100
10 (B2G)--O	-390.596	0	0	99.8	0.2	100
11 (EU)--O	-390.596	0	0	99.8	0.2	100
12 (EU)--O	-390.596	0	0	99.8	0.2	100
13 (A1G)--O	-390.596	0	0	99.9	0.1	100
14 (B2G)--O	-279.58	0	0	0.1	99.9	100
15 (EU)--O	-279.579	0	0	0.1	99.9	100
16 (EU)--O	-279.579	0	0	0.1	99.9	100
17 (A1G)--O	-279.579	0	0	0	100	100
18 (A2G)--O	-279.579	0	0	0	100	100
19 (EU)--O	-279.579	0	0	0	100	100
20 (EU)--O	-279.579	0	0	0	100	100
21 B1G)--O	-279.578	0	0	0	100	100
22 (EU)--O	-277.729	0	0	0	100	100
23 (EU)--O	-277.729	0	0	0	100	100
24 (A1G)--O	-277.729	0	0	0	100	100
25 (B1G)--O	-277.729	0	0	0	100	100
26 A2G)--O	-277.719	0	0	0	100	100
27 (EU)--O	-277.719	0	0	0	100	100
28 (EU)--O	-277.719	0	0	0	100	100
29 (B2G)--O	-277.719	0	0	0	100	100
30 (B1G)--O	-277.707	0	0	0	100	100
31 (EU)--O	-277.707	0	0	0	100	100
32 (EU)--O	-277.707	0	0	0	100	100
33 (A1G)--O	-277.707	0	0	0	100	100
34 (A2G)--O	-277.705	0	0	0	100	100
35 (EU)--O	-277.705	0	0	0	100	100
36 (EU)--O	-277.705	0	0	0	100	100
37 (B2G)--O	-277.705	0	0	0	100	100
38 (B1G)--O	-277.689	0	0	0	100	100
39 (EU)--O	-277.689	0	0	0	100	100
40 (EU)--O	-277.689	0	0	0	100	100
41 A1G)--O	-277.689	0	0	0	100	100
42 (A2G)--O	-277.679	0	0	0	100	100
43 (EU)--O	-277.679	0	0	0	100	100
44 (EU)--O	-277.679	0	0	0	100	100
45 (B2G)--O	-277.679	0	0	0	100	100
46 A1G)--O	-131.417	100	0	0	0	100
47 (A2U)--O	-87.748	100	0	0	0	100
48 (EU)--O	-87.471	100	0	0	0	100
49 (EU)--O	-87.471	100	0	0	0	100
50 (A1G)--O	-28.199	0.4	39.8	25.5	34.3	100
51 (EU)--O	-27.806	0.2	38.8	25.4	35.6	100
52 (EU)--O	-27.806	0.2	38.8	25.4	35.6	100
53 (B1G)--O	-27.033	0.2	59.6	0.8	39.5	100
54 (B2G)--O	-26.459	0	1.7	70.3	28	100
55 (EU)--O	-25.325	0	18.1	50.3	31.5	100
56 (EU)--O	-25.325	0	18.1	50.3	31.5	100



57 (A1G)--O	-24.463	0.1	16.7	49.8	33.4	100
58 (A1G)--O	-24.008	0.4	22.9	8.9	67.7	100
59 (EU)--O	-23.992	0.1	15	1.2	83.7	100
60 (EU)--O	-23.992	0.1	15	1.2	83.7	100
61 B1G)--O	-23.978	0.1	13.5	0	86.4	100
62 (A2G)--O	-21.799	0	2.7	6.5	90.8	100
63 (A1G)--O	-21.468	0.6	12.6	0.3	86.5	100
64 (EU)--O	-21.437	0.1	14.1	3.9	81.9	100
65 (EU)--O	-21.437	0.1	14.1	3.9	81.9	100
66 (EU)--O	-21.32	0	4.3	1.4	94.3	100
67 (EU)--O	-21.32	0	4.3	1.4	94.3	100
68 (B1G)--O	-21.312	0.5	19.3	0.6	79.6	100
69 (B2G)--O	-21.238	0	0	1.8	98.2	100
70 (A2G)--O	-20.328	0	5.8	9	85.2	100
71 (EU)--O	-19.603	0	7.4	18.9	73.7	100
72 (EU)--O	-19.603	0	7.4	18.9	73.7	100
73 (B1G)--O	-18.14	1.2	12.8	18.7	67.4	100
74 (A1G)--O	-18.028	2.1	11.7	0.3	85.9	100
75 (EU)--O	-17.852	0.2	10.9	0.3	88.6	100
76 (EU)--O	-17.852	0.2	10.9	0.3	88.6	100
77 (B2G)--O	-17.705	0.1	3.2	13.2	83.5	100
78 (B1G)--O	-17.566	0.8	4.2	11.8	83.2	100
79 (EU)--O	-16.904	0	6	3.7	90.3	100
80 (EU)--O	-16.904	0	6	3.7	90.3	100
81 B2G)--O	-16.816	2.3	31.5	22.3	43.8	100
82 (A2G)--O	-16.645	0	6.3	1.8	91.9	100
83 (A1G)--O	-15.809	4	9.2	1.4	85.3	100
84 (EU)--O	-15.627	0	18.8	13.1	68.1	100
85 (EU)--O	-15.627	0	18.8	13.1	68.1	100
86 B1G)--O	-15.214	14	14.8	5.2	65.9	100
87 (EU)--O	-15.19	0.3	15.2	19.6	64.9	100
88 (EU)--O	-15.19	0.3	15.2	19.6	64.9	100
89 (B2G)--O	-14.316	2.4	2.4	1.8	93.4	100
90 (A2G)--O	-14.304	0	27.2	15.8	57.1	100
91 B1G)--O	-14.033	50.7	14.1	0.5	34.7	100
92 (A1G)--O	-14.012	35.5	20.6	0.9	43.1	100
93 (EU)--O	-13.779	0	2.8	4.5	92.7	100
94 (EU)--O	-13.779	0	2.8	4.5	92.7	100
95 (EU)--O	-13.325	0.6	13.5	1	84.9	100
96 (EU)--O	-13.325	0.6	13.5	1	84.9	100
97 (EG)--O	-13.303	72.9	12.8	3.3	11.1	100
98 (EG)--O	-13.303	72.9	12.8	3.3	11.1	100
99 (A2U)--O	-13.275	0.4	26.2	18.4	55	100
100 (A2G)--O	-13.247	0	0.5	8	91.4	100
101 A1G)--O	-12.983	44.7	6.3	3	46.1	100
102 (B1G)--O	-12.917	16.7	7.7	1.2	74.4	100
103 (B2G)--O	-12.709	48.7	4.9	0.6	45.8	100
104 (A1G)--O	-12.651	17.1	1.4	3.4	78.1	100
105 (EU)--O	-12.61	0	1.2	1.6	97.2	100
106 (EU)--O	-12.61	0	1.2	1.6	97.2	100
107 (B2G)--O	-12.586	13.6	1.2	1.6	83.6	100

108 (EG)--O	-12.533	51.5	6.3	9.2	32.9	100
109 (EG)--O	-12.533	51.5	6.3	9.2	32.9	100
110 (A2G)--O	-12.314	0	0.6	4	95.4	100
111 (EU)--O	-12.228	0.3	5.7	4.5	89.5	100
112 (EU)--O	-12.228	0.3	5.7	4.5	89.5	100
113 (B2U)--O	-12.045	0	27.6	0	72.4	100
114 (B1G)--O	-11.908	9.3	0.9	4	85.8	100
115 (A1G)--O	-11.452	40.3	19.4	4.4	35.9	100
116 B1U)--O	-11.111	0	0.1	51.7	48.2	100
117 (B2G)--O	-10.734	0.4	0.1	1.8	97.7	100
118 (EU)--O	-10.653	0.1	2	2.5	95.4	100
119 (EU)--O	-10.653	0.1	2	2.5	95.4	100
120 (EG)--O	-10.562	0.8	2.7	13.9	82.6	100
121 (EG)--O	-10.562	0.8	2.7	13.9	82.6	100
122 (A2U)--O	-10.539	0.3	7.6	3.8	88.4	100
123 (A2G)--O	-10.442	0	2	1.1	96.9	100
124 (EU)--O	-10.318	4.2	36	3.1	56.7	100
125 (EU)--O	-10.318	4.2	36	3.1	56.7	100
126 A1G)--O	-10.268	0	1.8	3.2	95	100
127 (B2U)--O	-10.117	0	27.3	0	72.7	100
128 (B1G)--O	-9.91	1.4	1.1	2.9	94.6	100
129 (EU)--O	-9.904	1.9	14.9	6.8	76.4	100
130 (EU)--O	-9.904	1.9	14.9	6.8	76.4	100
131 (EG)--O	-9.348	1.7	22.1	21.9	54.2	100
132 (EG)--O	-9.348	1.7	22.1	21.9	54.2	100
133 (A1G)--O	-8.949	0.3	17.8	55	26.9	100
134 (A1U)--O	-8.201	0	0	0	99.9	100
135 (EU)--O	-8.193	0.2	18.5	50.7	30.6	100
136 (EU)--O	-8.193	0.2	18.5	50.7	30.6	100
137 (A2U)--O	-7.757	2.6	46.9	20.7	29.8	100
138 (B2G)--O	-7.697	0.6	12.7	62.2	24.5	100
139 (B1U)--O	-7.67	0	0	5.2	94.8	100
140 (EG)--O	-7.641	0	0.7	10	89.3	100
141 (EG)--O	-7.641	0	0.7	10	89.3	100
142 (A2U)--O	-7.48	0.2	6	39.4	54.4	100
143 (EG)--O	-7.446	1.3	27.7	1.3	69.7	100
144 (EG)--O	-7.446	1.3	27.7	1.3	69.7	100
145 (B2U)--O	-7.415	0	25.2	0	74.8	100
146 B1G)--O	-7.322	20.4	53.6	0.9	25.2	100
147 (A1U)--O	-5.632	0	0.1	0.1	99.8	100
148 (EG)--V	-3.442	0.3	13.3	19	67.4	100
149 (EG)--V	-3.442	0.3	13.3	19	67.4	100
150 (B1U)--V	-1.752	0	0	23.7	76.2	100
151 B2U)--V	-1.502	0	19	0	80.9	100
152 (A2U)--V	-1.343	6.2	1.1	5.5	87.3	100
153 (EG)--V	-1.196	0.1	5.3	3.6	91.1	100
154 (EG)--V	-1.196	0.1	5.3	3.6	91.1	100
155 (A1U)--V	0.076	0	0	0	100	100
156 (EG)--V	0.15	0	1.8	1	97.2	100
157 (EG)--V	0.15	0	1.8	1	97.2	100
158 (A2U)--V	0.384	62.4	7.1	2.4	28.1	100

159 (A1G)--V	0.613	72.6	16.7	0.3	10.5	100
160 (B2U)--V	0.785	0	19.4	0.1	80.5	100
161 B1U)--V	1.032	0	0.1	19.2	80.8	100
162 (A1G)--V	2.202	0.3	0.1	1.8	97.9	100
163 (EU)--V	2.234	18.7	2.8	1.7	76.9	100
164 (EU)--V	2.234	18.7	2.8	1.7	76.9	100
165 (B1G)--V	2.399	0	0	0.1	99.9	100
166 (EG)--V	2.455	0.1	14.3	16	69.6	100
167 (EG)--V	2.455	0.1	14.3	16	69.6	100
168 (EU)--V	2.478	49.1	6.2	1.3	43.5	100
169 (EU)--V	2.478	49.1	6.2	1.3	43.5	100
170 (A2U)--V	3.128	31.2	15.5	15.9	37.4	100
171 B2G)--V	3.264	0	1	0.2	98.8	100
172 (EU)--V	3.465	0	1.1	0.2	98.6	100
173 (EU)--V	3.465	0	1.1	0.2	98.6	100
174 (A1G)--V	3.542	28.8	0.4	10.9	59.9	100
175 (A2G)--V	3.71	0	0.7	0	99.3	100
176 (EU)--V	4.139	1.2	0.1	3.4	95.3	100
177 (EU)--V	4.139	1.2	0.1	3.4	95.3	100
178 (B2G)--V	4.154	0	0.1	5.4	94.5	100
179 (A1U)--V	4.205	0	0	0	100	100
180 (EG)--V	4.392	0	0.9	4.1	95	100
181 (EG)--V	4.392	0	0.9	4.1	95	100
182 (B1U)--V	4.402	0	0	4.6	95.4	100
183 (A1G)--V	4.474	33.3	1	0.4	65.4	100
184 (EU)--V	4.533	1	2	0.2	96.7	100
185 (EU)--V	4.533	1	2	0.2	96.7	100
186 B1G)--V	4.538	0	4.9	0.2	94.9	100
187 (A2G)--V	4.722	0	0.1	0	99.9	100
188 (B2G)--V	5.266	0.1	2.9	11.3	85.7	100
189 (EU)--V	5.272	5.4	8.9	4	81.6	100
190 (EU)--V	5.272	5.4	8.9	4	81.6	100
191 A1G)--V	5.512	0	0.7	1.3	97.9	100
192 (B1G)--V	5.566	0	28.6	3.4	68	100
193 (EU)--V	6.048	0.2	0.7	1.7	97.4	100
194 (EU)--V	6.048	0.2	0.7	1.7	97.4	100
195 (A2U)--V	6.115	85.8	3.5	1.5	9.1	100
196 A2G)--V	6.18	0	5.7	0.6	93.7	100
197 (B2G)--V	6.402	0	0.3	11.5	88.1	100
198 (EU)--V	6.418	0.8	0.2	5.7	93.3	100
199 (EU)--V	6.418	0.8	0.2	5.7	93.3	100
200 (A2G)--V	6.7	0	0.2	0	99.8	100
201 B1G)--V	6.729	0	1.9	0	98	100
202 (A1G)--V	7.094	7.6	9	20.6	62.7	100
203 (EU)--V	7.102	1.3	4.4	2	92.3	100
204 (EU)--V	7.102	1.3	4.4	2	92.3	100
205 (EU)--V	7.504	0.9	8.2	3.1	87.7	100
206 (EU)--V	7.504	0.9	8.2	3.1	87.7	100
207 (A1G)--V	7.589	5.7	0.6	3.4	90.2	100
208 (B1G)--V	8.211	0	0.4	0.1	99.6	100
209 (B2G)--V	8.216	0	0.8	3.7	95.4	100

210 (EU)--V	8.517	0.4	2.4	13.8	83.4	100
211 (EU)--V	8.517	0.4	2.4	13.8	83.4	100
212 (A1G)--V	8.747	0.3	2.1	2.4	95.2	100
213 (EU)--V	8.791	1.6	4.7	1.3	92.3	100
214 (EU)--V	8.791	1.6	4.7	1.3	92.3	100
215 (B2G)--V	9.08	0	4.2	24.6	71.2	100
216 B1G)--V	9.344	0	4.2	0.1	95.7	100
217 (B2G)--V	9.631	0	1.4	12.3	86.3	100
218 (EU)--V	10.008	2.4	3.8	17.1	76.7	100
219 (EU)--V	10.008	2.4	3.8	17.1	76.7	100
220 (A1G)--V	10.05	1.1	17.2	12.7	69.1	100
221 A2G)--V	10.116	0	6.8	8.4	84.7	100
222 (A2G)--V	10.928	0	0	0.8	99.2	100
223 (EU)--V	10.95	2.9	11	8.6	77.5	100
224 (EU)--V	10.95	2.9	11	8.6	77.5	100
225 (B1G)--V	11.054	0	19.4	8.2	72.3	100
226 (EU)--V	11.099	0.7	1.3	3.4	94.5	100
227 (EU)--V	11.099	0.7	1.3	3.4	94.5	100
228 (EU)--V	12.889	2.1	3.8	3.7	90.4	100
229 (EU)--V	12.889	2.1	3.8	3.7	90.4	100
230 (A2G)--V	13.099	0	0.2	6.2	93.5	100
231 (EG)--V	13.3	0	1.4	1.3	97.2	100
232 (EG)--V	13.3	0	1.4	1.3	97.2	100
233 (B2G)--V	13.311	0	0.3	0	99.6	100
234 (B2U)--V	13.516	0	0.4	0	99.6	100
235 (A2U)--V	13.626	3.8	0.2	0.7	95.4	100
236 (EU)--V	14.053	0.2	0.5	2.9	96.4	100
237 (EU)--V	14.053	0.2	0.5	2.9	96.4	100
238 (A1G)--V	14.154	0.7	3.9	0.8	94.5	100
239 (EG)--V	14.174	0	2.1	1.6	96.3	100
240 (EG)--V	14.174	0	2.1	1.6	96.3	100
241 B1G)--V	14.319	0	34	5	61	100
242 (A2G)--V	14.37	0	0.9	2.9	96.2	100
243 (B1U)--V	14.466	0	0	4.3	95.7	100
244 (B2G)--V	14.624	0	0.4	1.4	98.2	100
245 (EU)--V	14.649	0.2	0.4	0.3	99	100
246 (EU)--V	14.649	0.2	0.4	0.3	99	100
247 (B1G)--V	14.821	0	4.4	2	93.7	100
248 (EU)--V	14.892	0	0.5	1	98.5	100
249 (EU)--V	14.892	0	0.5	1	98.5	100
250 (B2U)--V	15	0	1.3	0.1	98.6	100
251 B2G)--V	15.09	0	0.9	1.6	97.5	100
252 (A2U)--V	15.111	10	1.4	1.4	87.2	100
253 (A1G)--V	15.16	1.8	1.3	12.9	83.9	100
254 (A2G)--V	15.175	0	0.2	0.8	98.9	100
255 (EG)--V	15.296	0	0.5	1.6	97.9	100
256 (EG)--V	15.296	0	0.5	1.6	97.9	100
257 (EU)--V	15.353	0.1	0.9	1.1	97.8	100
258 (EU)--V	15.353	0.1	0.9	1.1	97.8	100
259 (A1U)--V	15.437	0	0	0	100	100
260 (B1G)--V	15.439	0	25.2	1.1	73.8	100

261 A1G)--V	15.948	1.2	0.3	10.1	88.4	100
262 (EU)--V	15.95	0.3	16.3	15	68.5	100
263 (EU)--V	15.95	0.3	16.3	15	68.5	100
264 (A2G)--V	16.133	0	0.9	1.4	97.8	100
265 (B1G)--V	16.168	0	0.4	1.1	98.5	100
266 (EU)--V	16.177	0.2	0.8	0.5	98.5	100
267 (EU)--V	16.177	0.2	0.8	0.5	98.5	100
268 (A1G)--V	16.21	0.9	23	8.2	67.8	100
269 (B2G)--V	16.219	0	0.7	8.7	90.6	100
270 (B1U)--V	16.252	0	0	1.1	98.9	100
271 (EG)--V	16.474	0	3.6	0.6	95.8	100
272 (EG)--V	16.474	0	3.6	0.6	95.8	100
273 (A1G)--V	16.506	0.4	14	22.6	63	100
274 (EU)--V	16.525	1.3	23.2	10	65.5	100
275 (EU)--V	16.525	1.3	23.2	10	65.5	100
276 A2G)--V	16.82	0	1	3.2	95.9	100
277 (EU)--V	17.133	1.9	3.6	1.4	93.1	100
278 (EU)--V	17.133	1.9	3.6	1.4	93.1	100
279 (EG)--V	17.195	0	1.2	3.5	95.4	100
280 (EG)--V	17.195	0	1.2	3.5	95.4	100
281 A2U)--V	17.221	3	1.1	1.2	94.6	100
282 (EU)--V	17.286	1	1.5	14.1	83.3	100
283 (EU)--V	17.286	1	1.5	14.1	83.3	100
284 (B2U)--V	17.337	0	1.6	0	98.3	100
285 (B2G)--V	17.356	0	0.6	13.9	85.5	100
286 A1U)--V	17.392	0	0	0	100	100
287 (B1G)--V	17.773	0.1	12.1	9.2	78.7	100
288 (B1U)--V	18.094	0	0	2.3	97.7	100
289 (EG)--V	18.212	0	0.6	0.3	99.2	100
290 (EG)--V	18.212	0	0.6	0.3	99.2	100
291 A2U)--V	18.396	0.6	0.4	3.6	95.4	100
292 (A1G)--V	18.615	6	22.3	4.1	67.7	100
293 (B2U)--V	19.647	0	1	0	99	100
294 (EG)--V	19.713	0	1.2	1.6	97.1	100
295 (EG)--V	19.713	0	1.2	1.6	97.1	100
296 A1U)--V	19.911	0	0	0	100	100
297 (EU)--V	20.026	5.6	15.1	7.2	72.1	100
298 (EU)--V	20.026	5.6	15.1	7.2	72.1	100
299 (B1U)--V	20.458	0	0	3.3	96.6	100
300 (EG)--V	20.963	0.2	34.3	6.5	59	100
301 (EG)--V	20.963	0.2	34.3	6.5	59	100
302 (B2G)--V	21.223	0	0.2	3.4	96.4	100
303 (EU)--V	21.441	0.1	1.2	1.8	97	100
304 (EU)--V	21.441	0.1	1.2	1.8	97	100
305 (A1G)--V	21.575	0.1	0.5	1.1	98.4	100
306 A2U)--V	21.784	1.2	11.9	56.9	30.1	100
307 (B2G)--V	21.914	0	2.2	1.7	96.1	100
308 (EG)--V	22.07	0	2.5	0.5	96.9	100
309 (EG)--V	22.07	0	2.5	0.5	96.9	100
310 (A2G)--V	22.15	0	0.3	1.2	98.5	100
311 (EU)--V	22.223	0.1	0	1.1	98.8	100

312 (EU)--V	22.223	0.1	0	1.1	98.8	100
313 (A2G)--V	22.517	0	1.7	0.9	97.4	100
314 (EU)--V	22.665	0	0.9	0.3	98.8	100
315 (EU)--V	22.665	0	0.9	0.3	98.8	100
316 B1G)--V	22.708	0	1.2	0.6	98.2	100
317 (B2G)--V	22.853	0	6.5	10.6	82.9	100
318 (A1G)--V	23.08	0.5	9.7	7.4	82.4	100
319 (B2G)--V	23.087	0	5.4	0.9	93.6	100
320 (EU)--V	23.183	0.2	2	3.7	94.1	100
321 (EU)--V	23.183	0.2	2	3.7	94.1	100
322 (A2G)--V	23.576	0	0.5	8.3	91.2	100
323 (B2U)--V	23.585	0	69	0	31	100
324 (A1U)--V	23.631	0	0	0	100	100
325 (EU)--V	23.806	0.1	1	3.4	95.5	100
326 (EU)--V	23.806	0.1	1	3.4	95.5	100
327 (B1G)--V	23.808	0	0.5	0	99.5	100
328 (A1G)--V	23.892	2.5	2.7	26.3	68.5	100
329 (EG)--V	24.325	0.1	14.4	41.8	43.7	100
330 (EG)--V	24.325	0.1	14.4	41.8	43.7	100
331 B1U)--V	24.39	0	0	63.9	36	100
332 (B1G)--V	24.444	0	20.2	11.1	68.7	100
333 (A1G)--V	24.631	0.7	9.7	5.8	83.7	100
334 (EU)--V	24.691	0.3	3.3	7.1	89.3	100
335 (EU)--V	24.691	0.3	3.3	7.1	89.3	100
336 (EU)--V	25.058	0.4	9.7	5.2	84.7	100
337 (EU)--V	25.058	0.4	9.7	5.2	84.7	100
338 (A2G)--V	25.209	0	0	0	100	100
339 (B1G)--V	25.353	0	0.3	0.3	99.5	100
340 (EU)--V	25.725	0.4	0.1	4.2	95.3	100
341 (EU)--V	25.725	0.4	0.1	4.2	95.3	100
342 (B2G)--V	26.293	0	0.1	0.8	99.1	100
343 (A2U)--V	26.415	4.6	43.4	15.9	36.1	100
344 (A2G)--V	26.479	0	0	1.7	98.3	100
345 (EU)--V	26.517	0.1	1.2	2.6	96.2	100
346 (EU)--V	26.517	0.1	1.2	2.6	96.2	100
347 (B2G)--V	26.823	0	1	1.9	97.1	100
348 (B1G)--V	26.966	0	7.9	2.1	90	100
349 (EU)--V	27.165	0.4	6.3	3.4	89.9	100
350 (EU)--V	27.165	0.4	6.3	3.4	89.9	100
351 (EU)--V	27.574	0	5.7	5.7	88.6	100
352 (EU)--V	27.574	0	5.7	5.7	88.6	100
353 (A1G)--V	27.606	0	3.3	3.4	93.2	100
354 (A1G)--V	27.871	0.2	5.7	6.5	87.6	100
355 (B2G)--V	28.345	0	7.1	4	88.9	100
356 (EU)--V	28.792	0	2.3	3	94.7	100
357 (EU)--V	28.792	0	2.3	3	94.7	100
358 (A2G)--V	28.853	0	0.8	0.2	99	100
359 (A2G)--V	29.849	0	2.9	2.4	94.7	100
360 (B1G)--V	30.013	0	1	15.2	83.9	100
361 (EU)--V	30.104	0.1	1	0.8	98.2	100
362 (EU)--V	30.104	0.1	1	0.8	98.2	100

363 (B2G)--V	30.256	0	0.9	4.2	94.9	100
364 (B1G)--V	30.497	0	4.9	12.1	83	100
365 (A1G)--V	30.807	0.8	6.2	3.7	89.3	100
366 (EU)--V	30.925	0.1	5.6	3.3	90.9	100
367 (EU)--V	30.925	0.1	5.6	3.3	90.9	100
368 (B2G)--V	31.256	0	1.6	3.2	95.2	100
369 (A1G)--V	32.033	5.2	3.5	0.4	90.9	100
370 (B2U)--V	32.091	0	7.9	8.4	83.7	100
371 (EU)--V	32.221	1	6.3	4.7	88	100
372 (EU)--V	32.221	1	6.3	4.7	88	100
373 (A2G)--V	32.444	0	1.1	14.3	84.6	100
374 (EG)--V	32.49	0.1	5.4	14.4	80	100
375 (EG)--V	32.49	0.1	5.4	14.4	80	100
376 A2U)--V	33.123	0.2	0.9	10.9	88	100
377 (B1G)--V	33.173	0.3	13.2	8.7	77.8	100
378 (EU)--V	33.341	0.2	3.5	9.6	86.7	100
379 (EU)--V	33.341	0.2	3.5	9.6	86.7	100
380 (B2G)--V	33.624	0	1.7	1.9	96.4	100
381 A1U)--V	34.029	0	19.8	18.1	62.1	100
382 (EG)--V	34.062	0	8.7	9.7	81.5	100
383 (EG)--V	34.062	0	8.7	9.7	81.5	100
384 (B2U)--V	34.15	0	6.5	9.7	83.8	100
385 (EU)--V	34.39	0.2	1.7	12.4	85.7	100
386 (EU)--V	34.39	0.2	1.7	12.4	85.7	100
387 (A2G)--V	34.811	0	0.8	8.6	90.6	100
388 (B1U)--V	35.066	0	5.2	6.8	88	100
389 (EG)--V	35.16	0.2	5.2	7.3	87.3	100
390 (EG)--V	35.16	0.2	5.2	7.3	87.3	100
391 B1G)--V	35.245	0	0.4	4.3	95.3	100
392 (A1U)--V	35.396	0	3.6	5.7	90.6	100
393 (A2U)--V	35.895	4.2	27.3	17.2	51.2	100
394 (EG)--V	36.043	1.9	18.6	7.9	71.6	100
395 (EG)--V	36.043	1.9	18.6	7.9	71.6	100
396 A1G)--V	36.096	3.5	5.8	0.1	90.6	100
397 (EU)--V	36.164	0.1	3.8	0.6	95.5	100
398 (EU)--V	36.164	0.1	3.8	0.6	95.5	100
399 (B1G)--V	36.167	0	6	0.2	93.8	100
400 (EU)--V	36.97	0.3	6.7	0.2	92.8	100
401 (EU)--V	36.97	0.3	6.7	0.2	92.8	100
402 (B2U)--V	37.686	0	28.1	0.7	71.2	100
403 (A1G)--V	38.032	0.1	0.4	0	99.5	100
404 (A2G)--V	38.246	0	3	17.5	79.5	100
405 (B2G)--V	38.258	0	0.1	0.4	99.5	100
406 (EU)--V	38.283	0.1	1.1	1.6	97.2	100
407 (EU)--V	38.283	0.1	1.1	1.6	97.2	100
408 (B1G)--V	38.352	0	0.1	1.2	98.7	100
409 (EG)--V	38.492	0.2	4	5.9	90	100
410 (EG)--V	38.492	0.2	4	5.9	90	100
411 A2U)--V	38.509	0.5	2	2	95.5	100
412 (B2U)--V	38.581	0	0.2	0.7	99.2	100
413 (EG)--V	38.84	0.4	12.4	11.9	75.3	100

414 (EG)--V	38.84	0.4	12.4	11.9	75.3	100
415 (A2U)--V	39.067	2.3	10.2	0.8	86.7	100
416 B1U)--V	39.43	0	18.4	23.7	57.8	100
417 (B2U)--V	39.431	0	2.2	0.7	97	100
418 (EG)--V	39.705	0.2	5.8	2.9	91.1	100
419 (EG)--V	39.705	0.2	5.8	2.9	91.1	100
420 (A1U)--V	39.743	0	0	0	100	100
421 B1U)--V	39.804	0	4	5.6	90.4	100
422 (EG)--V	39.832	0.5	14.1	8.4	76.9	100
423 (EG)--V	39.832	0.5	14.1	8.4	76.9	100
424 (EU)--V	39.933	0	1.3	0.8	97.9	100
425 (EU)--V	39.933	0	1.3	0.8	97.9	100
426 A2G)--V	40.542	0	4.3	0.1	95.6	100
427 (A2U)--V	40.684	7.9	38.7	6.1	47.3	100
428 (A2G)--V	41.606	0	2.3	4.4	93.3	100
429 (B2G)--V	42.358	0	0.1	1.5	98.4	100
430 (EU)--V	42.41	0.2	4.9	0.2	94.7	100
431 (EU)--V	42.41	0.2	4.9	0.2	94.7	100
432 (A1G)--V	42.661	0.1	42	0.7	57.2	100
433 (EU)--V	42.924	0.7	12.8	2.5	83.9	100
434 (EU)--V	42.924	0.7	12.8	2.5	83.9	100
435 (A1G)--V	43.997	0.5	41.2	1.4	56.9	100
436 B1G)--V	44.328	0	33.8	2.7	63.5	100
437 (B2G)--V	45.391	0	0.2	19.7	80.1	100
438 (EU)--V	46.033	0.7	0.9	43.9	54.5	100
439 (EU)--V	46.033	0.7	0.9	43.9	54.5	100
440 (A1G)--V	46.323	1.1	0.9	54.3	43.8	100
441 B1G)--V	46.848	0	43.5	10.6	45.8	100
442 (EU)--V	47.148	0.2	34.8	4.1	60.9	100
443 (EU)--V	47.148	0.2	34.8	4.1	60.9	100
444 (B1U)--V	47.182	0	1.5	12.5	86.1	100
445 (A1G)--V	47.317	0.6	44.4	3.4	51.6	100
446 (EG)--V	47.501	0	2.5	10	87.5	100
447 (EG)--V	47.501	0	2.5	10	87.5	100
448 (A1U)--V	47.973	0	3.6	2.7	93.8	100
449 (B1G)--V	48.456	0	53.2	1.4	45.4	100
450 (B2G)--V	48.889	0	0.1	8.7	91.2	100
451 (EU)--V	48.968	0.1	21.5	2.6	75.8	100
452 (EU)--V	48.968	0.1	21.5	2.6	75.8	100
453 (A1G)--V	49.041	0.1	17.3	6.2	76.4	100
454 (EU)--V	49.211	0.1	1	21.5	77.5	100
455 (EU)--V	49.211	0.1	1	21.5	77.5	100
456 A2U)--V	49.382	0.5	10.6	25.2	63.8	100
457 (A2G)--V	49.44	0	0.5	0	99.5	100
458 (A1G)--V	49.784	0.6	19.9	38.5	41	100
459 (EU)--V	50.259	0	7.9	1.1	91	100
460 (EU)--V	50.259	0	7.9	1.1	91	100
461 B1G)--V	50.289	0	31.2	5.1	63.7	100
462 (EG)--V	50.474	0.4	15.9	17.6	66.1	100
463 (EG)--V	50.474	0.4	15.9	17.6	66.1	100
464 (A2G)--V	50.739	0	0	0	99.9	100



465 (B2G)--V	51.093	0	0	1.1	98.9	100
466 (EU)--V	51.187	0	0.5	1.1	98.4	100
467 (EU)--V	51.187	0	0.5	1.1	98.4	100
468 (A1G)--V	51.336	0	10.8	37.6	51.6	100
469 (B2U)--V	51.545	0	26.1	11.4	62.5	100
470 (EU)--V	51.663	1.7	5.9	18.1	74.2	100
471 (EU)--V	51.663	1.7	5.9	18.1	74.2	100
472 (B1G)--V	51.752	0	14.7	5.5	79.7	100
473 (B1G)--V	51.885	0	1.6	0.3	98.1	100
474 (EU)--V	52.188	2.7	13.5	9.4	74.4	100
475 (EU)--V	52.188	2.7	13.5	9.4	74.4	100
476 (EU)--V	52.768	14.9	31.7	0.6	52.9	100
477 (EU)--V	52.768	14.9	31.7	0.6	52.9	100
478 (A1G)--V	53.099	0.6	7.2	12.1	80.2	100
479 (A2G)--V	53.099	0	0	0.6	99.3	100
480 (B2G)--V	53.595	0	0.3	8.2	91.5	100
481 B2U)--V	53.798	0	27.2	14.5	58.3	100
482 (EU)--V	53.97	0	2.8	1.1	96.2	100
483 (EU)--V	53.97	0	2.8	1.1	96.2	100
484 (EU)--V	54.744	0.1	7.8	4.4	87.7	100
485 (EU)--V	54.744	0.1	7.8	4.4	87.7	100
486 A1G)--V	54.783	0	18.4	14	67.5	100
487 (EG)--V	55.039	1	28.3	17.6	53.1	100
488 (EG)--V	55.039	1	28.3	17.6	53.1	100
489 (B1G)--V	55.195	0	28.7	4.1	67.1	100
490 (A2G)--V	56.178	0	8.1	4.7	87.2	100
491 B1U)--V	56.184	0	2.4	29.1	68.5	100
492 (A1U)--V	56.262	0	24.8	11.2	64.1	100
493 (EG)--V	56.274	2.6	5.1	20.2	72.1	100
494 (EG)--V	56.274	2.6	5.1	20.2	72.1	100
495 (A2U)--V	56.285	0.3	4.8	20.8	74	100
496 B2G)--V	56.472	0	0.2	0.2	99.7	100
497 (EU)--V	56.752	0.1	0.8	1.7	97.4	100
498 (EU)--V	56.752	0.1	0.8	1.7	97.4	100
499 (A2G)--V	57	0	2.4	2.4	95.2	100
500 (EU)--V	57.037	0	2.2	4.1	93.7	100
501 (EU)--V	57.037	0	2.2	4.1	93.7	100
502 (B1G)--V	57.594	0	4.6	9.1	86.3	100
503 (B2G)--V	57.726	0	0.3	6.4	93.2	100
504 (EU)--V	57.984	0.1	0.8	3.4	95.7	100
505 (EU)--V	57.984	0.1	0.8	3.4	95.7	100
506 A1G)--V	58.262	0.8	4.6	0.8	93.8	100
507 (EG)--V	58.511	20.1	13.9	2	64	100
508 (EG)--V	58.511	20.1	13.9	2	64	100
509 (B1U)--V	58.855	0	9.8	13.2	77	100
510 (EG)--V	59.287	59.6	9.2	3	28.2	100
511 (EG)--V	59.287	59.6	9.2	3	28.2	100
512 (A1U)--V	59.743	0	5.6	5	89.4	100
513 (B2U)--V	59.858	0	1	0	99	100
514 (A2G)--V	59.922	0	0	0.4	99.5	100
515 (EU)--V	60.146	0	4.2	7.4	88.4	100

516 (EU)--V	60.146	0	4.2	7.4	88.4	100
517 (EG)--V	60.427	0.4	9	0.1	90.6	100
518 (EG)--V	60.427	0.4	9	0.1	90.6	100
519 (B1U)--V	60.537	0	6.5	1.5	92	100
520 (EG)--V	60.727	3.1	1.7	6.4	88.7	100
521 (EG)--V	60.727	3.1	1.7	6.4	88.7	100
522 (A2U)--V	60.805	0.3	31.6	6	62.1	100
523 (A2U)--V	60.9	0.1	11.4	0.9	87.6	100
524 (A1U)--V	61.027	0	0.2	4.9	94.9	100
525 (B2G)--V	61.129	0	0.2	11.5	88.3	100
526 (A2G)--V	61.211	0	3.4	1.4	95.2	100
527 (EU)--V	61.648	2.2	13.5	15.1	69.2	100
528 (EU)--V	61.648	2.2	13.5	15.1	69.2	100
529 (B1G)--V	61.873	0	36.1	16.6	47.4	100
530 (B2U)--V	61.929	0	2.4	1.2	96.4	100
531 (EG)--V	61.95	0	8.5	4.5	87	100
532 (EG)--V	61.95	0	8.5	4.5	87	100
533 (A1G)--V	62.75	0.1	1.2	17.6	81	100
534 (B2G)--V	63.64	5.7	4.1	7.8	82.4	100
535 (B1U)--V	63.781	0	18.2	1.7	80.1	100
536 (EU)--V	64.166	0.1	1.9	26.5	71.4	100
537 (EU)--V	64.166	0.1	1.9	26.5	71.4	100
538 (EG)--V	64.836	0.8	15.5	8.6	75.1	100
539 (EG)--V	64.836	0.8	15.5	8.6	75.1	100
540 (A2G)--V	64.846	0	0.1	0	99.9	100
541 (EU)--V	65.235	0	0.2	0.6	99.1	100
542 (EU)--V	65.235	0	0.2	0.6	99.1	100
543 (B2G)--V	65.477	0	2.2	24.3	73.5	100
544 (B1G)--V	65.536	0	1.8	0	98.1	100
545 (B2G)--V	66.201	0.6	5.2	7.2	86.9	100
546 (A1U)--V	67.036	0	2.6	6.7	90.6	100
547 (A2U)--V	67.186	0.2	8.8	19	72	100
548 (A1G)--V	67.214	1.9	16.2	1.1	80.8	100
549 (EU)--V	67.419	0.2	8.8	11.6	79.4	100
550 (EU)--V	67.419	0.2	8.8	11.6	79.4	100
551 (EG)--V	68.268	0	7.6	10	82.4	100
552 (EG)--V	68.268	0	7.6	10	82.4	100
553 (A1U)--V	69.367	0	13.5	12.3	74.2	100
554 (B1U)--V	69.487	0	12.4	8.3	79.3	100
555 (A1G)--V	70.733	2.6	19.2	35.3	42.9	100
556 (B1G)--V	70.737	0.6	56.8	4.7	37.9	100
557 (A2G)--V	70.948	0	0.6	0.2	99.1	100
558 (EG)--V	71.291	0.4	7.1	10.7	81.9	100
559 (EG)--V	71.291	0.4	7.1	10.7	81.9	100
560 (EU)--V	71.292	0	0.2	0.4	99.4	100
561 (EU)--V	71.292	0	0.2	0.4	99.4	100
562 (B2G)--V	71.347	0	0.3	0.1	99.6	100
563 (EU)--V	71.69	0.1	19.3	12.2	68.5	100
564 (EU)--V	71.69	0.1	19.3	12.2	68.5	100
565 (B1G)--V	71.917	0	0.6	2.2	97.2	100
566 (EU)--V	72.103	0.1	25.7	26.6	47.5	100

567 (EU)--V	72.103	0.1	25.7	26.6	47.5	100
568 (B1U)--V	72.134	0	0.2	4.1	95.7	100
569 (A1G)--V	72.189	1.6	13	24.7	60.7	100
570 (A2G)--V	72.217	0	2.9	2.1	95	100
571 (EU)--V	72.374	0	12.1	9.8	78.1	100
572 (EU)--V	72.374	0	12.1	9.8	78.1	100
573 (B1G)--V	72.493	0	28.3	4.7	67.1	100
574 (A1G)--V	73.202	7	9.5	3.4	80.2	100
575 (B2U)--V	73.272	0	15.9	30.8	53.3	100
576 A1U)--V	73.418	0	5.5	16.8	77.7	100
577 (EG)--V	73.474	0.2	10	22.2	67.5	100
578 (EG)--V	73.474	0.2	10	22.2	67.5	100
579 (EU)--V	73.603	0.1	42.4	13.7	43.9	100
580 (EU)--V	73.603	0.1	42.4	13.7	43.9	100
581 B1G)--V	73.607	0.2	30	4.3	65.5	100
582 (A1G)--V	73.864	0.4	55.5	18.4	25.7	100
583 (B2G)--V	74.633	0	0.2	7.4	92.3	100
584 (B2G)--V	75.028	0.1	4.3	20.4	75.2	100
585 (EU)--V	75.359	0	1.7	6.2	92.1	100
586 (EU)--V	75.359	0	1.7	6.2	92.1	100
587 (A2G)--V	75.763	0	0.7	6.3	93	100
588 (B1G)--V	75.949	1.5	50.3	4.2	44.1	100
589 (B2G)--V	76.275	0	0.1	0.4	99.4	100
590 (EU)--V	76.994	0	3.1	4.7	92.2	100
591 (EU)--V	76.994	0	3.1	4.7	92.2	100
592 (EU)--V	78.436	0.1	7.4	4.4	88.1	100
593 (EU)--V	78.436	0.1	7.4	4.4	88.1	100
594 (A2G)--V	78.657	0	1.2	2.4	96.4	100
595 (A1G)--V	78.885	0.3	21.4	25.2	53.1	100
596 (EU)--V	79.068	0.4	6.1	6.5	87.1	100
597 (EU)--V	79.068	0.4	6.1	6.5	87.1	100
598 (B2G)--V	80.491	0	0.1	8.1	91.8	100
599 (B1G)--V	80.83	0.9	7.1	6.3	85.7	100
600 (A2G)--V	81.455	0	0.2	0.1	99.7	100
601 A1G)--V	82.127	0.6	4.1	5.2	90.2	100
602 (EU)--V	82.15	0.1	10.1	10.8	79	100
603 (EU)--V	82.15	0.1	10.1	10.8	79	100
604 (A2G)--V	82.945	0	17.4	5.1	77.4	100
605 (B2G)--V	84.15	0	2.4	2.5	95.1	100
606 (EU)--V	84.594	0	1.1	5.7	93.2	100
607 (EU)--V	84.594	0	1.1	5.7	93.2	100
608 (EU)--V	87.004	0.2	7.2	19.8	72.8	100
609 (EU)--V	87.004	0.2	7.2	19.8	72.8	100
610 (B1G)--V	88.427	0.9	5.3	26	67.7	100
611 A1G)--V	90.283	0.4	4	55.3	40.3	100
612 (B2G)--V	90.714	0	1	1.8	97.2	100
613 (EU)--V	91.916	0	1.5	3	95.5	100
614 (EU)--V	91.916	0	1.5	3	95.5	100
615 (A2G)--V	92.639	0	6.1	11.2	82.7	100
616 A2G)--V	92.757	0	2.9	3	94.1	100
617 (EU)--V	94.691	0	5.6	4.5	89.9	100

618 (EU)--V	94.691	0	5.6	4.5	89.9	100
619 (B2G)--V	95.373	0	4	3.1	92.9	100

### PBE1PBE Exchange Correlation Functional

Orbital	Index	Energy,eV	Zn	NZn	Nmeso	Pc	Total
1	A1G)--O	-9458.24	100	0	0	0	100
2	(A1G)--O	-1152.17	100	0	0	0	100
3	(A2U)--O	-1014.74	100	0	0	0	100
4	(EU)--O	-1014.56	100	0	0	0	100
5	(EU)--O	-1014.56	100	0	0	0	100
6	B1G)--O	-392.295	0	99.8	0	0.2	100
7	(EU)--O	-392.295	0	99.9	0	0.1	100
8	(EU)--O	-392.295	0	99.9	0	0.1	100
9	(A1G)--O	-392.295	0	99.9	0	0.1	100
10	(B2G)--O	-392	0	0	99.8	0.2	100
11	(EU)--O	-392	0	0	99.8	0.2	100
12	(EU)--O	-392	0	0	99.8	0.2	100
13	(A1G)--O	-392	0	0	99.9	0.1	100
14	(B2G)--O	-280.635	0	0	0.1	99.9	100
15	(EU)--O	-280.635	0	0	0.1	99.9	100
16	(EU)--O	-280.635	0	0	0.1	99.9	100
17	(A2G)--O	-280.634	0	0	0	100	100
18	(A1G)--O	-280.634	0	0	0	100	100
19	(EU)--O	-280.634	0	0	0	100	100
20	(EU)--O	-280.634	0	0	0	100	100
21	B1G)--O	-280.634	0	0	0	100	100
22	(EU)--O	-278.79	0	0	0	100	100
23	(EU)--O	-278.79	0	0	0	100	100
24	(A1G)--O	-278.79	0	0	0	100	100
25	(B1G)--O	-278.79	0	0	0	100	100
26	A2G)--O	-278.779	0	0	0	100	100
27	(EU)--O	-278.779	0	0	0	100	100
28	(EU)--O	-278.779	0	0	0	100	100
29	(B2G)--O	-278.779	0	0	0	100	100
30	(B1G)--O	-278.759	0	0	0	100	100
31	(EU)--O	-278.759	0	0	0	100	100
32	(EU)--O	-278.759	0	0	0	100	100
33	(A1G)--O	-278.759	0	0	0	100	100
34	(A2G)--O	-278.757	0	0	0	100	100
35	(EU)--O	-278.757	0	0	0	100	100
36	(EU)--O	-278.757	0	0	0	100	100
37	(B2G)--O	-278.757	0	0	0	100	100
38	(B1G)--O	-278.738	0	0	0	100	100
39	(EU)--O	-278.738	0	0	0	100	100
40	(EU)--O	-278.738	0	0	0	100	100
41	A1G)--O	-278.738	0	0	0	100	100
42	(A2G)--O	-278.727	0	0	0	100	100

43 (EU)--O	-278.727	0	0	0	100	100
44 (EU)--O	-278.727	0	0	0	100	100
45 (B2G)--O	-278.727	0	0	0	100	100
46 A1G)--O	-132.286	100	0	0	0	100
47 (A2U)--O	-88.256	100	0	0	0	100
48 (EU)--O	-87.984	100	0	0	0	100
49 (EU)--O	-87.984	100	0	0	0	100
50 (A1G)--O	-28.246	0.4	40.2	25.6	33.8	100
51 (EU)--O	-27.847	0.2	39.2	25.5	35.2	100
52 (EU)--O	-27.847	0.2	39.2	25.5	35.2	100
53 (B1G)--O	-27.061	0.2	60.1	0.8	39	100
54 (B2G)--O	-26.473	0	1.7	70.7	27.6	100
55 (EU)--O	-25.318	0.1	18	50.7	31.2	100
56 (EU)--O	-25.318	0.1	18	50.7	31.2	100
57 (A1G)--O	-24.44	0.1	16.3	49.8	33.7	100
58 (A1G)--O	-23.988	0.4	23.9	9.9	65.9	100
59 (EU)--O	-23.974	0.1	15.4	1.3	83.2	100
60 (EU)--O	-23.974	0.1	15.4	1.3	83.2	100
61 B1G)--O	-23.96	0.1	13.9	0	86	100
62 (A2G)--O	-21.735	0	2.7	6.5	90.8	100
63 (A1G)--O	-21.402	0.6	12.7	0.3	86.4	100
64 (EU)--O	-21.368	0.1	14.6	3.8	81.5	100
65 (EU)--O	-21.368	0.1	14.6	3.8	81.5	100
66 (EU)--O	-21.25	0	4.2	1.4	94.4	100
67 (EU)--O	-21.25	0	4.2	1.4	94.4	100
68 (B1G)--O	-21.243	0.5	19.7	0.6	79.3	100
69 (B2G)--O	-21.165	0	0	1.8	98.2	100
70 (A2G)--O	-20.231	0	5.9	9.2	84.8	100
71 (EU)--O	-19.486	0	7.6	19.2	73.2	100
72 (EU)--O	-19.486	0	7.6	19.2	73.2	100
73 (B1G)--O	-17.99	1.3	13.5	18.2	67	100
74 (A1G)--O	-17.881	2	11.8	0.3	85.9	100
75 (EU)--O	-17.702	0.2	10.9	0.3	88.6	100
76 (EU)--O	-17.702	0.2	10.9	0.3	88.6	100
77 (B2G)--O	-17.553	0.1	3.2	13	83.7	100
78 (B1G)--O	-17.403	0.8	3.7	12.5	83.1	100
79 (EU)--O	-16.73	0	6	3.8	90.2	100
80 (EU)--O	-16.73	0	6	3.8	90.2	100
81 B2G)--O	-16.642	2.5	31.9	22.2	43.4	100
82 (A2G)--O	-16.466	0	6.5	1.9	91.6	100
83 (A1G)--O	-15.61	4.1	9.5	1.4	84.9	100
84 (EU)--O	-15.419	0	18.9	12.6	68.4	100
85 (EU)--O	-15.419	0	18.9	12.6	68.4	100
86 B1G)--O	-15.016	16.4	15.1	5.2	63.4	100
87 (EU)--O	-14.971	0.3	16.1	20.1	63.4	100
88 (EU)--O	-14.971	0.3	16.1	20.1	63.4	100
89 (B2G)--O	-14.089	2.9	2.5	1.9	92.7	100
90 (A2G)--O	-14.055	0	28.9	16.3	54.8	100
91 B1G)--O	-13.859	52.2	13.1	0.6	34.1	100
92 (A1G)--O	-13.805	39.2	20.3	0.8	39.7	100
93 (EU)--O	-13.535	0	2.7	4.7	92.6	100

94 (EU)--O	-13.535	0	2.7	4.7	92.6	100
95 (EG)--O	-13.149	78.5	10.9	2.4	8.2	100
96 (EG)--O	-13.149	78.5	10.9	2.4	8.2	100
97 (EU)--O	-13.076	0.6	13.5	0.9	85	100
98 (EU)--O	-13.076	0.6	13.5	0.9	85	100
99 (A2U)--O	-13.032	0.4	26.4	18.5	54.8	100
100 (A2G)--O	-12.989	0	0.5	8.4	91.1	100
101 A1G)--O	-12.78	47.9	5.4	2.5	44.2	100
102 (B1G)--O	-12.677	15.9	7.2	1.1	75.8	100
103 (B2G)--O	-12.561	53.2	5.1	0.8	40.9	100
104 (A1G)--O	-12.398	12.9	1.8	3.5	81.8	100
105 (EU)--O	-12.336	0	1.3	1.6	97.1	100
106 (EU)--O	-12.336	0	1.3	1.6	97.1	100
107 (EG)--O	-12.322	43.7	8.3	10.6	37.4	100
108 (EG)--O	-12.322	43.7	8.3	10.6	37.4	100
109 (B2G)--O	-12.317	3.3	0.2	1.4	95.1	100
110 (A2G)--O	-12.03	0	0.5	4.1	95.3	100
111 (EU)--O	-11.949	0.3	5.9	4.6	89.2	100
112 (EU)--O	-11.949	0.3	5.9	4.6	89.2	100
113 (B2U)--O	-11.778	0	27.7	0	72.2	100
114 (B1G)--O	-11.634	8.7	1	4.1	86.2	100
115 (A1G)--O	-11.174	37.1	20.7	4.9	37.3	100
116 B1U)--O	-10.816	0	0.1	51.9	48.1	100
117 (B2G)--O	-10.421	0.4	0.1	1.9	97.6	100
118 (EU)--O	-10.339	0.1	2.4	2.9	94.6	100
119 (EU)--O	-10.339	0.1	2.4	2.9	94.6	100
120 (EG)--O	-10.267	0.8	2.9	13.7	82.7	100
121 (EG)--O	-10.267	0.8	2.9	13.7	82.7	100
122 (A2U)--O	-10.245	0.3	7.7	3.8	88.3	100
123 (A2G)--O	-10.119	0	2	1.2	96.8	100
124 (EU)--O	-10.018	4	37.7	3.4	55	100
125 (EU)--O	-10.018	4	37.7	3.4	55	100
126 A1G)--O	-9.947	0	1.8	3.3	94.9	100
127 (B2U)--O	-9.813	0	27.6	0	72.4	100
128 (EU)--O	-9.586	1.6	13.3	6.7	78.4	100
129 (EU)--O	-9.586	1.6	13.3	6.7	78.4	100
130 (B1G)--O	-9.583	1.4	1.3	2.9	94.5	100
131 (EG)--O	-9.01	1.6	22.4	22.2	53.8	100
132 (EG)--O	-9.01	1.6	22.4	22.2	53.8	100
133 (A1G)--O	-8.682	0.3	17.6	55	27.1	100
134 (EU)--O	-7.898	0.2	18.8	50.8	30.2	100
135 (EU)--O	-7.898	0.2	18.8	50.8	30.2	100
136 A1U)--O	-7.831	0	0	0	99.9	100
137 (B2G)--O	-7.392	0.6	13	62.5	24	100
138 (A2U)--O	-7.377	2.4	46	19	32.5	100
139 (B1U)--O	-7.292	0	0	5.2	94.8	100
140 (EG)--O	-7.26	0	0.6	10	89.4	100
141 (EG)--O	-7.26	0	0.6	10	89.4	100
142 (A2U)--O	-7.079	0.2	7.2	40.9	51.7	100
143 (EG)--O	-7.066	1.2	27.6	1.3	69.9	100
144 (EG)--O	-7.066	1.2	27.6	1.3	69.9	100

145 (B2U)--O	-7.032	0	25	0	75	100
146 B1G)--O	-7.026	19.9	54.4	0.9	24.8	100
147 (A1U)--O	-5.133	0	0.1	0.1	99.8	100
148 (EG)--V	-2.753	0.3	13.3	18.9	67.5	100
149 (EG)--V	-2.753	0.3	13.3	18.9	67.5	100
150 (B1U)--V	-0.997	0	0	23.3	76.6	100
151 B2U)--V	-0.739	0	18.8	0	81.1	100
152 (A2U)--V	-0.586	7.3	0.9	5.5	86.4	100
153 (EG)--V	-0.427	0.1	5.2	3.5	91.2	100
154 (EG)--V	-0.427	0.1	5.2	3.5	91.2	100
155 (A1U)--V	0.87	0	0	0	100	100
156 (EG)--V	0.948	0	1.8	1	97.2	100
157 (EG)--V	0.948	0	1.8	1	97.2	100
158 (A2U)--V	0.996	65.6	7.9	1.4	25.1	100
159 (A1G)--V	1.224	76.5	13.5	0.2	9.7	100
160 (B2U)--V	1.608	0	19.5	0.1	80.4	100
161 B1U)--V	1.869	0	0.1	19.4	80.6	100
162 (EU)--V	2.849	57.4	5.7	2.1	34.8	100
163 (EU)--V	2.849	57.4	5.7	2.1	34.8	100
164 (A1G)--V	2.925	0.3	0	1.7	98	100
165 (EU)--V	3.095	17.8	1.5	0.3	80.4	100
166 (EU)--V	3.095	17.8	1.5	0.3	80.4	100
167 (B1G)--V	3.134	0	0	0.1	99.9	100
168 (EG)--V	3.331	0.1	14.3	15.9	69.7	100
169 (EG)--V	3.331	0.1	14.3	15.9	69.7	100
170 (A2U)--V	3.85	36	13.1	15.2	35.7	100
171 B2G)--V	3.975	0	0.9	0.1	98.9	100
172 (EU)--V	4.192	0	1.1	0.2	98.7	100
173 (EU)--V	4.192	0	1.1	0.2	98.7	100
174 (A1G)--V	4.289	26.6	0.4	10.4	62.6	100
175 (A2G)--V	4.461	0	0.7	0.1	99.3	100
176 (EU)--V	4.869	0.9	0.1	3.2	95.8	100
177 (EU)--V	4.869	0.9	0.1	3.2	95.8	100
178 (B2G)--V	4.896	0	0.1	4.7	95.2	100
179 (A1U)--V	5.105	0	0	0	100	100
180 (A1G)--V	5.212	32.8	1.2	0.3	65.7	100
181 (EG)--V	5.297	0	0.9	4.2	94.9	100
182 (EG)--V	5.297	0	0.9	4.2	94.9	100
183 (EU)--V	5.298	0.7	1.9	0.2	97.2	100
184 (EU)--V	5.298	0.7	1.9	0.2	97.2	100
185 (B1U)--V	5.303	0	0	4.6	95.4	100
186 B1G)--V	5.311	0	4.2	0.1	95.7	100
187 (A2G)--V	5.476	0	0.1	0	99.9	100
188 (EU)--V	6.062	4.8	9.5	4.5	81.1	100
189 (EU)--V	6.062	4.8	9.5	4.5	81.1	100
190 (B2G)--V	6.072	0.1	2.9	12.1	84.9	100
191 A1G)--V	6.342	0	0.7	1.4	97.9	100
192 (B1G)--V	6.428	0	29.4	3.4	67.2	100
193 (A2U)--V	6.852	82.2	4.7	2.1	11	100
194 (EU)--V	6.891	0.2	0.7	1.8	97.4	100
195 (EU)--V	6.891	0.2	0.7	1.8	97.4	100

196 A2G)--V	7.027	0	5.6	0.5	93.8	100
197 (B2G)--V	7.242	0	0.3	11.4	88.3	100
198 (EU)--V	7.262	0.7	0.2	5.5	93.6	100
199 (EU)--V	7.262	0.7	0.2	5.5	93.6	100
200 (A2G)--V	7.531	0	0.2	0	99.8	100
201 B1G)--V	7.584	0	1.8	0	98.2	100
202 (EU)--V	7.937	1.2	3.9	1.7	93.2	100
203 (EU)--V	7.937	1.2	3.9	1.7	93.2	100
204 (A1G)--V	7.949	7	9.2	21.8	62.1	100
205 (EU)--V	8.376	0.9	8.8	3.1	87.2	100
206 (EU)--V	8.376	0.9	8.8	3.1	87.2	100
207 (A1G)--V	8.426	5.1	0.6	3	91.3	100
208 (B1G)--V	9.058	0	0.4	0.1	99.6	100
209 (B2G)--V	9.106	0	0.8	3.4	95.7	100
210 (EU)--V	9.396	0.4	2.3	13.9	83.5	100
211 (EU)--V	9.396	0.4	2.3	13.9	83.5	100
212 (A1G)--V	9.612	0.3	2.1	2.4	95.2	100
213 (EU)--V	9.663	1.5	5.1	1.6	91.9	100
214 (EU)--V	9.663	1.5	5.1	1.6	91.9	100
215 (B2G)--V	9.966	0	4	24.9	71.1	100
216 B1G)--V	10.219	0	4.2	0.1	95.7	100
217 (B2G)--V	10.52	0	1.6	11.9	86.4	100
218 (EU)--V	10.896	2.3	3.7	17.2	76.8	100
219 (EU)--V	10.896	2.3	3.7	17.2	76.8	100
220 (A1G)--V	10.96	1.1	17.5	12.6	68.8	100
221 A2G)--V	11.072	0	6.9	8.4	84.7	100
222 (A2G)--V	11.871	0	0	0.8	99.1	100
223 (EU)--V	11.881	2.6	11	8.5	77.9	100
224 (EU)--V	11.881	2.6	11	8.5	77.9	100
225 (B1G)--V	11.952	0	19.6	8.3	72.1	100
226 (EU)--V	12.048	0.7	1.3	3.4	94.5	100
227 (EU)--V	12.048	0.7	1.3	3.4	94.5	100
228 (EU)--V	13.851	1.9	3.7	3.5	90.8	100
229 (EU)--V	13.851	1.9	3.7	3.5	90.8	100
230 (A2G)--V	14.074	0	0.2	6	93.7	100
231 B2G)--V	14.256	0	0.3	0	99.6	100
232 (EG)--V	14.305	0	1.4	1.3	97.3	100
233 (EG)--V	14.305	0	1.4	1.3	97.3	100
234 (B2U)--V	14.525	0	0.4	0	99.6	100
235 (A2U)--V	14.63	3.6	0.2	0.7	95.5	100
236 (EU)--V	15.037	0.2	0.5	2.7	96.6	100
237 (EU)--V	15.037	0.2	0.5	2.7	96.6	100
238 (A1G)--V	15.086	0.7	3.9	0.8	94.6	100
239 (EG)--V	15.181	0	2	1.6	96.4	100
240 (EG)--V	15.181	0	2	1.6	96.4	100
241 B1G)--V	15.227	0	34.1	5	61	100
242 (A2G)--V	15.359	0	0.9	2.9	96.3	100
243 (B1U)--V	15.471	0	0	4.2	95.8	100
244 (EU)--V	15.583	0.2	0.5	0.3	99	100
245 (EU)--V	15.583	0.2	0.5	0.3	99	100
246 B2G)--V	15.636	0	0.3	1.3	98.4	100



247 (B1G)--V	15.766	0	5.1	1.8	93.2	100
248 (EU)--V	15.844	0	0.5	1.2	98.3	100
249 (EU)--V	15.844	0	0.5	1.2	98.3	100
250 (B2U)--V	16.009	0	1.3	0.1	98.6	100
251 B2G)--V	16.041	0	0.9	1.6	97.4	100
252 (A2U)--V	16.097	9.3	1.5	1.4	87.9	100
253 (A2G)--V	16.115	0	0.3	0.8	98.9	100
254 (A1G)--V	16.138	1.7	1.1	12.1	85	100
255 (EG)--V	16.307	0	0.5	1.5	98	100
256 (EG)--V	16.307	0	0.5	1.5	98	100
257 (EU)--V	16.325	0.2	0.9	1	97.9	100
258 (EU)--V	16.325	0.2	0.9	1	97.9	100
259 (B1G)--V	16.428	0	24.8	1	74.2	100
260 (A1U)--V	16.448	0	0	0	100	100
261 (EU)--V	16.945	0.3	17.5	14.3	67.9	100
262 (EU)--V	16.945	0.3	17.5	14.3	67.9	100
263 (A1G)--V	16.945	1.4	2	6.8	89.7	100
264 (A2G)--V	17.134	0	0.9	1.4	97.7	100
265 (A1G)--V	17.142	0.7	23.1	9.5	66.6	100
266 B1G)--V	17.163	0	0.5	1.2	98.3	100
267 (EU)--V	17.173	0.2	1	0.6	98.2	100
268 (EU)--V	17.173	0.2	1	0.6	98.2	100
269 (B2G)--V	17.225	0	0.7	7.9	91.4	100
270 (B1U)--V	17.267	0	0	1.1	98.9	100
271 (EU)--V	17.49	1.3	23.5	8.9	66.3	100
272 (EU)--V	17.49	1.3	23.5	8.9	66.3	100
273 (EG)--V	17.495	0	3.5	0.6	95.8	100
274 (EG)--V	17.495	0	3.5	0.6	95.8	100
275 (A1G)--V	17.529	0.6	11.7	23.7	64	100
276 A2G)--V	17.849	0	1	3.2	95.8	100
277 (EU)--V	18.168	1.9	3.6	1.5	93	100
278 (EU)--V	18.168	1.9	3.6	1.5	93	100
279 (EG)--V	18.226	0	1.1	3.4	95.5	100
280 (EG)--V	18.226	0	1.1	3.4	95.5	100
281 A2U)--V	18.235	2.8	1.1	1.2	94.9	100
282 (EU)--V	18.354	1	1.4	14.6	83	100
283 (EU)--V	18.354	1	1.4	14.6	83	100
284 (B2U)--V	18.366	0	1.6	0	98.4	100
285 (B2G)--V	18.412	0	0.6	14.1	85.3	100
286 A1U)--V	18.419	0	0	0	100	100
287 (B1G)--V	18.882	0.1	11.7	9.3	79	100
288 (B1U)--V	19.12	0	0	2.3	97.6	100
289 (EG)--V	19.241	0	0.5	0.3	99.2	100
290 (EG)--V	19.241	0	0.5	0.3	99.2	100
291 A2U)--V	19.428	0.6	0.4	3.4	95.7	100
292 (A1G)--V	19.636	5.7	22	4.1	68.1	100
293 (B2U)--V	20.672	0	1	0	99	100
294 (EG)--V	20.744	0	1.1	1.5	97.4	100
295 (EG)--V	20.744	0	1.1	1.5	97.4	100
296 A1U)--V	20.937	0	0	0	100	100
297 (EU)--V	20.992	5.4	14.7	7.2	72.7	100

298 (EU)--V	20.992	5.4	14.7	7.2	72.7	100
299 (B1U)--V	21.483	0	0	3.3	96.7	100
300 (EG)--V	22.02	0.2	33.3	6.3	60.2	100
301 (EG)--V	22.02	0.2	33.3	6.3	60.2	100
302 (B2G)--V	22.252	0	0.2	3.3	96.5	100
303 (EU)--V	22.442	0.1	1.3	1.8	96.9	100
304 (EU)--V	22.442	0.1	1.3	1.8	96.9	100
305 (A1G)--V	22.557	0.1	0.4	1	98.5	100
306 A2U)--V	22.869	1.1	11.9	57.6	29.4	100
307 (B2G)--V	22.929	0	2.1	1.5	96.4	100
308 (EG)--V	23.111	0	2.9	0.6	96.4	100
309 (EG)--V	23.111	0	2.9	0.6	96.4	100
310 (A2G)--V	23.158	0	0.3	1.3	98.4	100
311 (EU)--V	23.219	0.1	0	1	98.9	100
312 (EU)--V	23.219	0.1	0	1	98.9	100
313 (A2G)--V	23.48	0	1.7	0.8	97.5	100
314 (EU)--V	23.644	0	0.9	0.3	98.8	100
315 (EU)--V	23.644	0	0.9	0.3	98.8	100
316 B1G)--V	23.684	0	1.2	0.6	98.2	100
317 (B2G)--V	23.906	0	5.9	11.9	82.2	100
318 (A1G)--V	24.038	0.5	9.9	7.6	82	100
319 (B2G)--V	24.093	0	6.9	0.5	92.6	100
320 (EU)--V	24.177	0.2	2.3	3.9	93.7	100
321 (EU)--V	24.177	0.2	2.3	3.9	93.7	100
322 (A2G)--V	24.629	0	0.5	8.2	91.3	100
323 (A1U)--V	24.662	0	0	0	100	100
324 (B2U)--V	24.668	0	69.5	0	30.4	100
325 (B1G)--V	24.767	0	0.5	0	99.5	100
326 (EU)--V	24.775	0.1	0.9	3.4	95.6	100
327 (EU)--V	24.775	0.1	0.9	3.4	95.6	100
328 (A1G)--V	24.914	2.3	2.4	24.9	70.4	100
329 (EG)--V	25.386	0.1	14.3	42.2	43.3	100
330 (EG)--V	25.386	0.1	14.3	42.2	43.3	100
331 B1G)--V	25.433	0	20.1	11.2	68.6	100
332 (B1U)--V	25.475	0	0	64.2	35.8	100
333 (A1G)--V	25.618	0.8	10.2	6.3	82.7	100
334 (EU)--V	25.75	0.3	3.3	6.8	89.7	100
335 (EU)--V	25.75	0.3	3.3	6.8	89.7	100
336 (EU)--V	26.06	0.4	10.1	5.5	84	100
337 (EU)--V	26.06	0.4	10.1	5.5	84	100
338 (A2G)--V	26.227	0	0	0	100	100
339 (B1G)--V	26.371	0	0.3	0.3	99.4	100
340 (EU)--V	26.751	0.4	0.2	4.5	94.9	100
341 (EU)--V	26.751	0.4	0.2	4.5	94.9	100
342 (B2G)--V	27.342	0	0.2	1	98.8	100
343 (A2U)--V	27.456	4.6	43.6	15.9	35.9	100
344 (EU)--V	27.567	0.1	1.5	2.7	95.7	100
345 (EU)--V	27.567	0.1	1.5	2.7	95.7	100
346 A2G)--V	27.577	0	0	1.7	98.3	100
347 (B2G)--V	27.851	0	0.9	1.8	97.4	100
348 (B1G)--V	27.961	0	7.8	2.2	90	100

349 (EU)--V	28.151	0.3	5.6	3.1	91.1	100
350 (EU)--V	28.151	0.3	5.6	3.1	91.1	100
351 (EU)--V	28.58	0	5.4	5.6	88.9	100
352 (EU)--V	28.58	0	5.4	5.6	88.9	100
353 (A1G)--V	28.627	0	3.3	3.4	93.3	100
354 (A1G)--V	28.845	0.2	5.5	6.6	87.7	100
355 (B2G)--V	29.336	0	7.2	4	88.8	100
356 (EU)--V	29.804	0	2.4	3	94.6	100
357 (EU)--V	29.804	0	2.4	3	94.6	100
358 (A2G)--V	29.843	0	0.7	0.2	99.1	100
359 (A2G)--V	30.876	0	3	2.6	94.4	100
360 (B1G)--V	31.054	0	0.9	15.1	84	100
361 (EU)--V	31.125	0.1	0.9	0.8	98.2	100
362 (EU)--V	31.125	0.1	0.9	0.8	98.2	100
363 (B2G)--V	31.305	0	0.9	4.1	94.9	100
364 (B1G)--V	31.515	0	4.8	12.1	83.1	100
365 (A1G)--V	31.837	0.8	6.2	3.7	89.4	100
366 (EU)--V	31.942	0.1	5.6	3.5	90.8	100
367 (EU)--V	31.942	0.1	5.6	3.5	90.8	100
368 (B2G)--V	32.284	0	1.8	3.2	95	100
369 (B2U)--V	32.965	0	8	8.4	83.6	100
370 (A1G)--V	33.048	5.3	3.7	0.4	90.6	100
371 (EU)--V	33.259	1	6.3	4.7	88	100
372 (EU)--V	33.259	1	6.3	4.7	88	100
373 (EG)--V	33.372	0.1	5.5	14.6	79.8	100
374 (EG)--V	33.372	0.1	5.5	14.6	79.8	100
375 (A2G)--V	33.492	0	1	14.4	84.6	100
376 A2U)--V	34.012	0.2	0.9	11.1	87.8	100
377 (B1G)--V	34.257	0.4	14.1	8.7	76.9	100
378 (EU)--V	34.342	0.2	3.5	9.8	86.4	100
379 (EU)--V	34.342	0.2	3.5	9.8	86.4	100
380 (B2G)--V	34.643	0	1.7	1.9	96.4	100
381 A1U)--V	34.905	0	19.6	18	62.4	100
382 (EG)--V	34.949	0	8.7	9.6	81.6	100
383 (EG)--V	34.949	0	8.7	9.6	81.6	100
384 (B2U)--V	35.04	0	6.6	9.6	83.7	100
385 (EU)--V	35.388	0.2	1.6	12.2	86	100
386 (EU)--V	35.388	0.2	1.6	12.2	86	100
387 (A2G)--V	35.814	0	0.8	8.8	90.4	100
388 (B1U)--V	35.96	0	5.2	6.9	87.9	100
389 (EG)--V	36.054	0.2	5.2	7.3	87.3	100
390 (EG)--V	36.054	0.2	5.2	7.3	87.3	100
391 B1G)--V	36.249	0	0.4	4.3	95.3	100
392 (A1U)--V	36.291	0	3.6	5.7	90.6	100
393 (A2U)--V	36.811	4.3	27.7	17.2	50.9	100
394 (EG)--V	36.949	1.9	18.6	7.9	71.6	100
395 (EG)--V	36.949	1.9	18.6	7.9	71.6	100
396 A1G)--V	37.171	3.5	5.9	0.1	90.5	100
397 (B1G)--V	37.217	0	6.1	0.2	93.7	100
398 (EU)--V	37.226	0.1	3.7	0.7	95.5	100
399 (EU)--V	37.226	0.1	3.7	0.7	95.5	100

400 (EU)--V	37.985	0.3	6.8	0.2	92.8	100
401 (EU)--V	37.985	0.3	6.8	0.2	92.8	100
402 (B2U)--V	38.596	0	28.1	0.7	71.2	100
403 (A1G)--V	39.058	0.1	0.4	0	99.4	100
404 (A2G)--V	39.264	0	3	17.7	79.3	100
405 (B2G)--V	39.284	0	0.1	0.4	99.5	100
406 (EU)--V	39.311	0.1	1.1	1.6	97.2	100
407 (EU)--V	39.311	0.1	1.1	1.6	97.2	100
408 (B1G)--V	39.385	0	0.1	1.2	98.7	100
409 (EG)--V	39.412	0.1	3.9	5.8	90.1	100
410 (EG)--V	39.412	0.1	3.9	5.8	90.1	100
411 A2U)--V	39.429	0.5	1.9	2	95.5	100
412 (B2U)--V	39.5	0	0.2	0.7	99.2	100
413 (EG)--V	39.761	0.4	12.5	11.9	75.2	100
414 (EG)--V	39.761	0.4	12.5	11.9	75.2	100
415 (A2U)--V	39.992	2.4	10.4	0.8	86.5	100
416 B1U)--V	40.35	0	18.5	23.9	57.6	100
417 (B2U)--V	40.36	0	2.2	0.7	97	100
418 (EG)--V	40.636	0.2	5.5	2.8	91.5	100
419 (EG)--V	40.636	0.2	5.5	2.8	91.5	100
420 (A1U)--V	40.673	0	0	0	100	100
421 B1U)--V	40.733	0	3.8	5.4	90.8	100
422 (EG)--V	40.764	0.5	14.3	8.5	76.6	100
423 (EG)--V	40.764	0.5	14.3	8.5	76.6	100
424 (EU)--V	40.974	0	1.4	0.8	97.8	100
425 (EU)--V	40.974	0	1.4	0.8	97.8	100
426 A2G)--V	41.574	0	4.3	0	95.6	100
427 (A2U)--V	41.619	7.9	38.6	6.1	47.4	100
428 (A2G)--V	42.664	0	2.4	4.4	93.2	100
429 (B2G)--V	43.405	0	0.1	1.6	98.3	100
430 (EU)--V	43.417	0.2	5.2	0.2	94.4	100
431 (EU)--V	43.417	0.2	5.2	0.2	94.4	100
432 (A1G)--V	43.671	0.1	42.3	0.7	57	100
433 (EU)--V	43.921	0.7	12.5	2.5	84.4	100
434 (EU)--V	43.921	0.7	12.5	2.5	84.4	100
435 (A1G)--V	44.988	0.5	40.8	1.6	57.1	100
436 B1G)--V	45.302	0	34	2.7	63.3	100
437 (B2G)--V	46.333	0	0.2	19.5	80.3	100
438 (EU)--V	47.03	0.7	1	44	54.3	100
439 (EU)--V	47.03	0.7	1	44	54.3	100
440 (A1G)--V	47.337	1.1	0.9	54.3	43.7	100
441 B1G)--V	47.87	0	43.4	10.6	45.9	100
442 (B1U)--V	48.14	0	1.4	12.5	86	100
443 (EU)--V	48.163	0.2	34.7	4.2	61	100
444 (EU)--V	48.163	0.2	34.7	4.2	61	100
445 (A1G)--V	48.332	0.6	44.2	3.5	51.7	100
446 (EG)--V	48.462	0	2.4	10.1	87.5	100
447 (EG)--V	48.462	0	2.4	10.1	87.5	100
448 (A1U)--V	48.937	0	3.6	2.7	93.8	100
449 (B1G)--V	49.47	0	53	1.2	45.8	100
450 (B2G)--V	49.927	0	0.1	8.6	91.3	100

451 (EU)--V	50.012	0.1	21.6	2.5	75.8	100
452 (EU)--V	50.012	0.1	21.6	2.5	75.8	100
453 (A1G)--V	50.056	0.1	15.5	8.5	75.8	100
454 (EU)--V	50.221	0.1	0.8	21.8	77.3	100
455 (EU)--V	50.221	0.1	0.8	21.8	77.3	100
456 A2U)--V	50.35	0.5	10.6	25.2	63.8	100
457 (A2G)--V	50.514	0	0.5	0	99.5	100
458 (A1G)--V	50.81	0.5	20.3	37.7	41.5	100
459 (EU)--V	51.303	0	7.7	1.1	91.2	100
460 (EU)--V	51.303	0	7.7	1.1	91.2	100
461 B1G)--V	51.325	0	31.1	5.1	63.8	100
462 (EG)--V	51.453	0.4	15.8	17.6	66.2	100
463 (EG)--V	51.453	0.4	15.8	17.6	66.2	100
464 (A2G)--V	51.803	0	0.1	0	99.9	100
465 (B2G)--V	52.146	0	0	1.1	98.9	100
466 (EU)--V	52.241	0	0.5	1.2	98.3	100
467 (EU)--V	52.241	0	0.5	1.2	98.3	100
468 (A1G)--V	52.399	0	10.7	37.1	52.2	100
469 (B2U)--V	52.532	0	26	11.4	62.6	100
470 (EU)--V	52.735	1.6	5.6	16.7	76.1	100
471 (EU)--V	52.735	1.6	5.6	16.7	76.1	100
472 (B1G)--V	52.784	0	14.5	5.5	80	100
473 (B1G)--V	52.967	0	1.3	0.2	98.5	100
474 (EU)--V	53.252	2.3	13.4	9.3	75.1	100
475 (EU)--V	53.252	2.3	13.4	9.3	75.1	100
476 (EU)--V	53.876	15.6	32.3	0.6	51.4	100
477 (EU)--V	53.876	15.6	32.3	0.6	51.4	100
478 (A1G)--V	54.146	0.5	7.1	11.7	80.6	100
479 (A2G)--V	54.153	0	0	0.6	99.3	100
480 (B2G)--V	54.663	0	0.4	8	91.6	100
481 B2U)--V	54.782	0	27.4	14.6	58	100
482 (EU)--V	55.032	0	2.5	1	96.5	100
483 (EU)--V	55.032	0	2.5	1	96.5	100
484 (EU)--V	55.812	0.1	8.3	4.6	87	100
485 (EU)--V	55.812	0.1	8.3	4.6	87	100
486 A1G)--V	55.861	0	18.5	13.9	67.5	100
487 (EG)--V	56.036	0.8	28.3	17.8	53.1	100
488 (EG)--V	56.036	0.8	28.3	17.8	53.1	100
489 (B1G)--V	56.269	0	28.8	4.2	67	100
490 (B1U)--V	57.181	0	2.4	29.1	68.6	100
491 A2G)--V	57.238	0	8.2	4.7	87.1	100
492 (A1U)--V	57.266	0	24.7	11.1	64.2	100
493 (A2U)--V	57.281	0.3	4.8	20.8	74	100
494 (EG)--V	57.282	2	5.2	20.2	72.6	100
495 (EG)--V	57.282	2	5.2	20.2	72.6	100
496 B2G)--V	57.539	0	0.2	0.1	99.7	100
497 (EU)--V	57.829	0.1	0.8	1.9	97.2	100
498 (EU)--V	57.829	0.1	0.8	1.9	97.2	100
499 (EU)--V	58.09	0	2.1	3.8	94	100
500 (EU)--V	58.09	0	2.1	3.8	94	100
501 A2G)--V	58.112	0	2.4	2.4	95.3	100

502 (B1G)--V	58.652	0	4.5	9	86.5	100
503 (B2G)--V	58.781	0	0.4	6.5	93.1	100
504 (EU)--V	59.048	0.1	0.8	3.5	95.7	100
505 (EU)--V	59.048	0.1	0.8	3.5	95.7	100
506 A1G)--V	59.332	0.8	4.6	0.8	93.7	100
507 (EG)--V	59.578	10.3	13.4	2.7	73.6	100
508 (EG)--V	59.578	10.3	13.4	2.7	73.6	100
509 (B1U)--V	59.851	0	9.8	13.2	77	100
510 (EG)--V	60.601	66.9	9.5	2	21.6	100
511 (EG)--V	60.601	66.9	9.5	2	21.6	100
512 (A1U)--V	60.75	0	5.7	5	89.3	100
513 (B2U)--V	60.864	0	1	0	99	100
514 (A2G)--V	60.974	0	0	0.5	99.5	100
515 (EU)--V	61.213	0	4.3	7.7	88	100
516 (EU)--V	61.213	0	4.3	7.7	88	100
517 (EG)--V	61.441	0.7	9	0.1	90.3	100
518 (EG)--V	61.441	0.7	9	0.1	90.3	100
519 (B1U)--V	61.549	0	6.5	1.5	92	100
520 (EG)--V	61.76	5.4	2.1	6.5	86	100
521 (EG)--V	61.76	5.4	2.1	6.5	86	100
522 (A2U)--V	61.812	0.3	32.9	5.8	61	100
523 (A2U)--V	61.912	0.1	9.6	1.1	89.2	100
524 (A1U)--V	62.04	0	0.2	4.9	94.9	100
525 (B2G)--V	62.216	0	0.2	11.5	88.3	100
526 A2G)--V	62.314	0	3.6	1.4	95	100
527 (EU)--V	62.733	2.2	13.4	14.7	69.6	100
528 (EU)--V	62.733	2.2	13.4	14.7	69.6	100
529 (B2U)--V	62.94	0	2.4	1.2	96.4	100
530 (B1G)--V	62.958	0	35.9	16.6	47.5	100
531 (EG)--V	62.964	0	8.4	4.6	87	100
532 (EG)--V	62.964	0	8.4	4.6	87	100
533 (A1G)--V	63.789	0.1	1.3	17.6	81	100
534 (B1U)--V	64.803	0	18.2	1.7	80.1	100
535 (B2G)--V	64.935	5.4	3.1	12.3	79.2	100
536 (EU)--V	65.211	0.1	2	26.7	71.2	100
537 (EU)--V	65.211	0.1	2	26.7	71.2	100
538 (EG)--V	65.861	0.9	15.6	8.6	74.9	100
539 (EG)--V	65.861	0.9	15.6	8.6	74.9	100
540 (A2G)--V	65.908	0	0.1	0	99.9	100
541 (EU)--V	66.296	0	0.2	0.6	99.1	100
542 (EU)--V	66.296	0	0.2	0.6	99.1	100
543 (B2G)--V	66.532	0	2.1	23.8	74.1	100
544 (B1G)--V	66.587	0	1.8	0	98.1	100
545 (B2G)--V	67.345	0.8	5.9	9.2	84.1	100
546 A1U)--V	68.063	0	2.7	6.7	90.6	100
547 (A2U)--V	68.216	0.2	8.9	19	72	100
548 (A1G)--V	68.342	1.7	15.9	0.9	81.4	100
549 (EU)--V	68.498	0.2	8.8	11.7	79.3	100
550 (EU)--V	68.498	0.2	8.8	11.7	79.3	100
551 (EG)--V	69.3	0	7.6	10	82.4	100
552 (EG)--V	69.3	0	7.6	10	82.4	100

553 (A1U)--V	70.4	0	13.5	12.3	74.1	100
554 (B1U)--V	70.522	0	12.4	8.3	79.3	100
555 (A1G)--V	71.865	2.5	19.9	35.2	42.4	100
556 B1G)--V	71.929	0.6	56.8	4.7	37.9	100
557 (A2G)--V	72.031	0	0.6	0.2	99.2	100
558 (EG)--V	72.336	0.4	7.1	10.7	81.8	100
559 (EG)--V	72.336	0.4	7.1	10.7	81.8	100
560 (EU)--V	72.357	0	0.2	0.3	99.5	100
561 (EU)--V	72.357	0	0.2	0.3	99.5	100
562 (B2G)--V	72.431	0	0.3	0.1	99.6	100
563 (EU)--V	72.821	0.1	20.2	12.6	67.1	100
564 (EU)--V	72.821	0.1	20.2	12.6	67.1	100
565 (B1G)--V	73.051	0	0.5	1.8	97.6	100
566 B1U)--V	73.179	0	0.2	4.1	95.7	100
567 (EU)--V	73.235	0.1	25.3	26.5	48.2	100
568 (EU)--V	73.235	0.1	25.3	26.5	48.2	100
569 (A1G)--V	73.327	1.3	13.4	24.5	60.8	100
570 (A2G)--V	73.327	0	3.2	2.3	94.5	100
571 (EU)--V	73.482	0	12.4	10	77.5	100
572 (EU)--V	73.482	0	12.4	10	77.5	100
573 (B1G)--V	73.59	0	29	4.9	66	100
574 (B2U)--V	74.32	0	15.9	30.8	53.2	100
575 (A1G)--V	74.457	6.3	15	7.4	71.4	100
576 A1U)--V	74.465	0	5.5	16.8	77.7	100
577 (EG)--V	74.523	0.3	10	22.3	67.5	100
578 (EG)--V	74.523	0.3	10	22.3	67.5	100
579 (EU)--V	74.718	0.1	43	13.4	43.5	100
580 (EU)--V	74.718	0.1	43	13.4	43.5	100
581 B1G)--V	74.75	0.1	31.1	4.6	64.1	100
582 (A1G)--V	75.028	0.9	55.7	16.6	26.9	100
583 (B2G)--V	75.772	0	0.3	7.4	92.3	100
584 (B2G)--V	76.177	0.2	4.4	20	75.4	100
585 (EU)--V	76.493	0	1.5	6.1	92.4	100
586 (EU)--V	76.493	0	1.5	6.1	92.4	100
587 (A2G)--V	76.914	0	0.7	6.1	93.2	100
588 (B1G)--V	77.176	1.7	48.6	3.9	45.9	100
589 (B2G)--V	77.424	0	0.1	0.5	99.4	100
590 (EU)--V	78.139	0	3.3	4.8	91.9	100
591 (EU)--V	78.139	0	3.3	4.8	91.9	100
592 (EU)--V	79.536	0.1	7.5	4.3	88.1	100
593 (EU)--V	79.536	0.1	7.5	4.3	88.1	100
594 (A2G)--V	79.791	0	1.2	2.3	96.5	100
595 (A1G)--V	79.973	0.3	21.4	25.3	53	100
596 (EU)--V	80.191	0.3	6	6.7	87	100
597 (EU)--V	80.191	0.3	6	6.7	87	100
598 (B2G)--V	81.596	0	0.1	8.2	91.7	100
599 (B1G)--V	82.073	1	7.2	6.4	85.4	100
600 (A2G)--V	82.558	0	0.2	0.1	99.7	100
601 (EU)--V	83.28	0.1	10.1	10.7	79	100
602 (EU)--V	83.28	0.1	10.1	10.7	79	100
603 (A1G)--V	83.293	0.6	4.1	5.1	90.2	100

604 (A2G)--V	84.114	0	17.9	5.3	76.8	100
605 (B2G)--V	85.315	0	2.4	2.5	95.1	100
606 (EU)--V	85.752	0	1.2	5.8	93	100
607 (EU)--V	85.752	0	1.2	5.8	93	100
608 (EU)--V	88.157	0.2	7.1	19.8	72.9	100
609 (EU)--V	88.157	0.2	7.1	19.8	72.9	100
610 (B1G)--V	89.631	1	5.4	26.1	67.5	100
611 A1G)--V	91.449	0.4	3.9	55.4	40.3	100
612 (B2G)--V	91.875	0	1	1.8	97.2	100
613 (EU)--V	93.082	0	1.4	3	95.5	100
614 (EU)--V	93.082	0	1.4	3	95.5	100
615 (A2G)--V	93.811	0	5.6	10.5	84	100
616 A2G)--V	93.936	0	3.3	3.5	93.2	100
617 (EU)--V	95.872	0	5.6	4.5	89.8	100
618 (EU)--V	95.872	0	5.6	4.5	89.8	100
619 (B2G)--V	96.556	0	4	3.1	92.8	100

### B98 Exchange Correlation Functional

Orbital	Index	E, eV	Zn	NZn	Nmeso	Pc	Total	
	1 A1G)--O	-9451.02		100	0	0	0	100
	2 (A1G)--O	-1150.46		100	0	0	0	100
	3 (A2U)--O	-1013.64		100	0	0	0	100
	4 (EU)--O	-1013.46		100	0	0	0	100
	5 (EU)--O	-1013.46		100	0	0	0	100
	6 B1G)--O	-391.116		0	99.8	0	0.2	100
	7 (EU)--O	-391.116		0	99.9	0	0.1	100
	8 (EU)--O	-391.116		0	99.9	0	0.1	100
	9 (A1G)--O	-391.116		0	99.9	0	0.1	100
	10 (B2G)--O	-390.855		0	0	99.8	0.2	100
	11 (EU)--O	-390.855		0	0	99.8	0.2	100
	12 (EU)--O	-390.855		0	0	99.8	0.2	100
	13 (A1G)--O	-390.855		0	0	99.9	0.1	100
	14 (B2G)--O	-279.952		0	0	0.1	99.9	100
	15 (EU)--O	-279.952		0	0	0	99.9	100
	16 (EU)--O	-279.952		0	0	0	99.9	100
	17 (A1G)--O	-279.951		0	0	0	100	100
	18 (A2G)--O	-279.951		0	0	0	100	100
	19 (EU)--O	-279.951		0	0	0	100	100
	20 (EU)--O	-279.951		0	0	0	100	100
	21 B1G)--O	-279.951		0	0	0	100	100
	22 (EU)--O	-278.042		0	0	0	100	100
	23 (EU)--O	-278.042		0	0	0	100	100
	24 (A1G)--O	-278.042		0	0	0	100	100
	25 (B1G)--O	-278.042		0	0	0	100	100
	26 A2G)--O	-278.035		0	0	0	100	100
	27 (EU)--O	-278.035		0	0	0	100	100
	28 (EU)--O	-278.035		0	0	0	100	100
	29 (B2G)--O	-278.035		0	0	0	100	100



30 (B1G)--O	-278.027	0	0	0	100	100
31 (EU)--O	-278.027	0	0	0	100	100
32 (EU)--O	-278.027	0	0	0	100	100
33 (A1G)--O	-278.027	0	0	0	100	100
34 (A2G)--O	-278.022	0	0	0	100	100
35 (EU)--O	-278.022	0	0	0	100	100
36 (EU)--O	-278.022	0	0	0	100	100
37 (B2G)--O	-278.022	0	0	0	100	100
38 (B1G)--O	-278.01	0	0	0	100	100
39 (EU)--O	-278.01	0	0	0	100	100
40 (EU)--O	-278.01	0	0	0	100	100
41 A1G)--O	-278.01	0	0	0	100	100
42 (A2G)--O	-278	0	0	0	100	100
43 (B2G)--O	-278	0	0	0	100	100
44 (EU)--O	-278	0	0	0	100	100
45 (EU)--O	-278	0	0	0	100	100
46 A1G)--O	-131.123	100	0	0	0	100
47 (A2U)--O	-87.414	100	0	0	0	100
48 (EU)--O	-87.135	100	0	0	0	100
49 (EU)--O	-87.135	100	0	0	0	100
50 (A1G)--O	-27.729	0.4	39.8	25.9	34	100
51 (EU)--O	-27.335	0.2	38.8	25.7	35.3	100
52 (EU)--O	-27.335	0.2	38.8	25.7	35.3	100
53 (B1G)--O	-26.558	0.2	59.7	0.8	39.3	100
54 (B2G)--O	-25.984	0	1.7	70.6	27.7	100
55 (EU)--O	-24.844	0	18.2	50.4	31.3	100
56 (EU)--O	-24.844	0	18.2	50.4	31.3	100
57 (A1G)--O	-23.981	0.1	16.9	49.9	33	100
58 (A1G)--O	-23.525	0.3	22.9	8.7	68	100
59 (EU)--O	-23.508	0.1	15	1.2	83.7	100
60 (EU)--O	-23.508	0.1	15	1.2	83.7	100
61 B1G)--O	-23.494	0.1	13.4	0	86.4	100
62 (A2G)--O	-21.301	0	2.6	6.3	91	100
63 (A1G)--O	-20.974	0.6	12.6	0.3	86.5	100
64 (EU)--O	-20.945	0.1	14	3.8	82.1	100
65 (EU)--O	-20.945	0.1	14	3.8	82.1	100
66 (EU)--O	-20.829	0	4.4	1.3	94.2	100
67 (EU)--O	-20.829	0	4.4	1.3	94.2	100
68 (B1G)--O	-20.821	0.5	19.3	0.6	79.7	100
69 (B2G)--O	-20.748	0	0	1.8	98.2	100
70 (A2G)--O	-19.82	0	5.8	9.1	85	100
71 (EU)--O	-19.084	0	7.4	18.9	73.7	100
72 (EU)--O	-19.084	0	7.4	18.9	73.7	100
73 (B1G)--O	-17.618	1.3	13.2	17.9	67.7	100
74 (A1G)--O	-17.516	2	11.8	0.3	85.9	100
75 (EU)--O	-17.343	0.2	11	0.3	88.5	100
76 (EU)--O	-17.343	0.2	11	0.3	88.5	100
77 (B2G)--O	-17.194	0.1	3.1	13.1	83.8	100
78 (B1G)--O	-17.043	0.7	3.8	12.7	82.8	100
79 (EU)--O	-16.383	0	5.8	3.8	90.4	100
80 (EU)--O	-16.383	0	5.8	3.8	90.4	100

81 B2G)--O	-16.271	2.4	31.7	22.4	43.4	100
82 (A2G)--O	-16.126	0	6.1	1.9	92.1	100
83 (A1G)--O	-15.283	4.1	9.4	1.4	85.2	100
84 (EU)--O	-15.091	0	18.2	12.1	69.7	100
85 (EU)--O	-15.091	0	18.2	12.1	69.7	100
86 B1G)--O	-14.693	15.3	15.1	5.2	64.4	100
87 (EU)--O	-14.641	0.3	15.9	20.2	63.5	100
88 (EU)--O	-14.641	0.3	15.9	20.2	63.5	100
89 (B2G)--O	-13.799	2.5	2.4	1.8	93.3	100
90 (A2G)--O	-13.741	0	27.2	15.4	57.4	100
91 B1G)--O	-13.542	51.6	13.3	0.5	34.6	100
92 (A1G)--O	-13.492	38.3	20	0.8	40.9	100
93 (EU)--O	-13.257	0	2.7	4.5	92.8	100
94 (EU)--O	-13.257	0	2.7	4.5	92.8	100
95 (EG)--O	-12.821	78.9	10.7	2.4	8	100
96 (EG)--O	-12.821	78.9	10.7	2.4	8	100
97 (EU)--O	-12.794	0.6	13.6	1	84.8	100
98 (EU)--O	-12.794	0.6	13.6	1	84.8	100
99 (A2G)--O	-12.728	0	0.5	8.1	91.4	100
100 (A2U)--O	-12.701	0.4	26.3	18.4	55	100
101 A1G)--O	-12.489	46.4	5.9	2.8	44.9	100
102 (B1G)--O	-12.398	15.9	7.8	1.2	75.1	100
103 (B2G)--O	-12.246	51.9	5	0.7	42.4	100
104 (A1G)--O	-12.127	13.1	1.7	3.7	81.4	100
105 (EU)--O	-12.089	0	1.2	1.5	97.2	100
106 (EU)--O	-12.089	0	1.2	1.5	97.2	100
107 (B2G)--O	-12.073	7.1	0.5	1.4	90.9	100
108 (EG)--O	-12.002	43.2	8.4	10.6	37.8	100
109 (EG)--O	-12.002	43.2	8.4	10.6	37.8	100
110 (A2G)--O	-11.788	0	0.6	4.1	95.3	100
111 (EU)--O	-11.694	0.3	5.7	4.6	89.4	100
112 (EU)--O	-11.694	0.3	5.7	4.6	89.4	100
113 (B2U)--O	-11.464	0	27.7	0	72.3	100
114 (B1G)--O	-11.381	8.8	0.9	4	86.3	100
115 (A1G)--O	-10.896	37.9	20.8	4.6	36.8	100
116 B1U)--O	-10.515	0	0.1	51.7	48.3	100
117 (B2G)--O	-10.212	0.4	0.1	1.8	97.7	100
118 (EU)--O	-10.129	0.1	1.9	2.5	95.6	100
119 (EU)--O	-10.129	0.1	1.9	2.5	95.6	100
120 (EG)--O	-9.972	0.8	2.8	13.7	82.7	100
121 (EG)--O	-9.972	0.8	2.8	13.7	82.7	100
122 (A2U)--O	-9.95	0.3	7.6	3.8	88.3	100
123 (A2G)--O	-9.914	0	1.9	1.2	96.9	100
124 (EU)--O	-9.773	3.7	34.3	3	59	100
125 (EU)--O	-9.773	3.7	34.3	3	59	100
126 A1G)--O	-9.745	0	1.7	3.2	95.1	100
127 (B2U)--O	-9.525	0	27.5	0	72.5	100
128 (B1G)--O	-9.385	1.4	1.2	3	94.4	100
129 (EU)--O	-9.36	2.1	17.2	7.1	73.6	100
130 (EU)--O	-9.36	2.1	17.2	7.1	73.6	100
131 (EG)--O	-8.742	1.6	22.3	22	54.1	100

132 (EG)--O	-8.742	1.6	22.3	22	54.1	100
133 (A1G)--O	-8.404	0.3	17.4	55.6	26.7	100
134 (EU)--O	-7.643	0.2	18.3	50.6	30.9	100
135 (EU)--O	-7.643	0.2	18.3	50.6	30.9	100
136 A1U)--O	-7.587	0	0	0	99.9	100
137 (B2G)--O	-7.149	0.5	12.7	62	24.7	100
138 (A2U)--O	-7.138	2.5	46.2	19.5	31.7	100
139 (B1U)--O	-7.052	0	0	5.2	94.8	100
140 (EG)--O	-7.021	0	0.7	10	89.3	100
141 (EG)--O	-7.021	0	0.7	10	89.3	100
142 (A2U)--O	-6.846	0.2	6.8	40.5	52.5	100
143 (EG)--O	-6.828	1.2	27.7	1.3	69.7	100
144 (EG)--O	-6.828	1.2	27.7	1.3	69.7	100
145 (B2U)--O	-6.795	0	25.2	0	74.8	100
146 B1G)--O	-6.785	19.9	54.1	0.9	25.1	100
147 (A1U)--O	-4.966	0	0.1	0.1	99.8	100
148 (EG)--V	-2.702	0.3	13.3	18.9	67.5	100
149 (EG)--V	-2.702	0.3	13.3	18.9	67.5	100
150 (B1U)--V	-0.988	0	0	23.6	76.4	100
151 B2U)--V	-0.741	0	18.9	0	81.1	100
152 (A2U)--V	-0.593	7.5	0.8	5.5	86.1	100
153 (EG)--V	-0.432	0.1	5.2	3.6	91.2	100
154 (EG)--V	-0.432	0.1	5.2	3.6	91.2	100
155 (A1U)--V	0.85	0	0	0	100	100
156 (EG)--V	0.926	0	1.8	1	97.2	100
157 (EG)--V	0.926	0	1.8	1	97.2	100
158 (A2U)--V	0.945	65.3	8.2	1.3	25.2	100
159 (A1G)--V	1.153	76.8	13.4	0.2	9.6	100
160 (B2U)--V	1.57	0	19.4	0.1	80.5	100
161 B1U)--V	1.822	0	0.1	19.2	80.7	100
162 (EU)--V	2.776	55.5	5.6	2	36.9	100
163 (EU)--V	2.776	55.5	5.6	2	36.9	100
164 (A1G)--V	2.843	0.4	0	1.6	98	100
165 (EU)--V	3.013	19.4	1.6	0.3	78.7	100
166 (EU)--V	3.013	19.4	1.6	0.3	78.7	100
167 (B1G)--V	3.047	0	0	0.1	99.9	100
168 (EG)--V	3.257	0.1	14.2	16	69.7	100
169 (EG)--V	3.257	0.1	14.2	16	69.7	100
170 (A2U)--V	3.777	35	13.3	15.4	36.3	100
171 B2G)--V	3.874	0	0.9	0.1	99	100
172 (EU)--V	4.09	0	1	0.2	98.8	100
173 (EU)--V	4.09	0	1	0.2	98.8	100
174 (A1G)--V	4.222	24.5	0.4	10	65.1	100
175 (A2G)--V	4.357	0	0.6	0.1	99.3	100
176 (EU)--V	4.77	0.8	0.1	3	96.1	100
177 (EU)--V	4.77	0.8	0.1	3	96.1	100
178 (B2G)--V	4.809	0	0.1	4.2	95.7	100
179 (A1U)--V	5.012	0	0	0	100	100
180 (A1G)--V	5.117	35	1.2	0.5	63.3	100
181 (EU)--V	5.2	0.6	1.6	0.1	97.7	100
182 (EU)--V	5.2	0.6	1.6	0.1	97.7	100

183 (EG)--V	5.201	0	0.9	4.1	95	100
184 (EG)--V	5.201	0	0.9	4.1	95	100
185 (B1G)--V	5.204	0	3.8	0.1	96.1	100
186 B1U)--V	5.21	0	0	4.6	95.4	100
187 (A2G)--V	5.358	0	0.1	0	99.9	100
188 (EU)--V	6.002	5.1	10.3	4.8	79.9	100
189 (EU)--V	6.002	5.1	10.3	4.8	79.9	100
190 (B2G)--V	6.031	0.1	3	12.8	84	100
191 A1G)--V	6.305	0	0.6	1.2	98.2	100
192 (B1G)--V	6.334	0	30.1	3.5	66.4	100
193 (A2U)--V	6.77	82.9	4.5	2	10.6	100
194 (EU)--V	6.831	0.2	0.6	1.9	97.2	100
195 (EU)--V	6.831	0.2	0.6	1.9	97.2	100
196 A2G)--V	6.953	0	5.8	0.6	93.6	100
197 (B2G)--V	7.163	0	0.3	12	87.7	100
198 (EU)--V	7.193	0.7	0.2	5.5	93.6	100
199 (EU)--V	7.193	0.7	0.2	5.5	93.6	100
200 (A2G)--V	7.458	0	0.2	0	99.8	100
201 B1G)--V	7.511	0	1.7	0	98.2	100
202 (A1G)--V	7.84	7.4	9.3	22	61.3	100
203 (EU)--V	7.869	1.2	4.2	2	92.7	100
204 (EU)--V	7.869	1.2	4.2	2	92.7	100
205 (EU)--V	8.28	0.9	8.5	3	87.6	100
206 (EU)--V	8.28	0.9	8.5	3	87.6	100
207 (A1G)--V	8.348	4.9	0.6	2.6	91.9	100
208 (B1G)--V	8.975	0	0.4	0.1	99.5	100
209 (B2G)--V	8.992	0	1	4.7	94.3	100
210 (EU)--V	9.272	0.4	2.1	13.7	83.7	100
211 (EU)--V	9.272	0.4	2.1	13.7	83.7	100
212 (A1G)--V	9.507	0.3	2.1	2.3	95.3	100
213 (EU)--V	9.566	1.4	5.1	2.2	91.3	100
214 (EU)--V	9.566	1.4	5.1	2.2	91.3	100
215 (B2G)--V	9.867	0	4	24.1	71.8	100
216 B1G)--V	10.083	0	4	0.1	95.9	100
217 (B2G)--V	10.447	0	1.4	12.2	86.3	100
218 (EU)--V	10.814	2.4	3.7	16.9	77	100
219 (EU)--V	10.814	2.4	3.7	16.9	77	100
220 (A1G)--V	10.824	1.1	17.3	12.9	68.7	100
221 A2G)--V	10.898	0	6.7	8.4	84.9	100
222 (A2G)--V	11.697	0	0	0.8	99.1	100
223 (EU)--V	11.728	2.8	11	8.8	77.3	100
224 (EU)--V	11.728	2.8	11	8.8	77.3	100
225 (B1G)--V	11.829	0	19.6	8.3	72.2	100
226 (EU)--V	11.871	0.7	1.4	3.4	94.5	100
227 (EU)--V	11.871	0.7	1.4	3.4	94.5	100
228 (EU)--V	13.689	1.9	3.6	3.4	91.1	100
229 (EU)--V	13.689	1.9	3.6	3.4	91.1	100
230 (A2G)--V	13.889	0	0.2	6	93.8	100
231 B2G)--V	14.048	0	0.3	0	99.7	100
232 (EG)--V	14.159	0	1.4	1.3	97.2	100
233 (EG)--V	14.159	0	1.4	1.3	97.2	100

234 (B2U)--V	14.378	0	0.4	0	99.6	100
235 (A2U)--V	14.484	3.6	0.2	0.7	95.5	100
236 (EU)--V	14.806	0.2	0.5	2.5	96.8	100
237 (EU)--V	14.806	0.2	0.5	2.5	96.8	100
238 (A1G)--V	14.933	0.7	4.4	0.9	94	100
239 (EG)--V	15.032	0	2	1.6	96.4	100
240 (EG)--V	15.032	0	2	1.6	96.4	100
241 B1G)--V	15.115	0	34.1	5	60.9	100
242 (A2G)--V	15.127	0	0.8	2.6	96.6	100
243 (B1U)--V	15.317	0	0	4.2	95.8	100
244 (B2G)--V	15.394	0	0.3	1.1	98.5	100
245 (EU)--V	15.421	0.2	0.5	0.4	99	100
246 (EU)--V	15.421	0.2	0.5	0.4	99	100
247 (B1G)--V	15.6	0	4	2	94	100
248 (EU)--V	15.639	0	0.5	1.3	98.2	100
249 (EU)--V	15.639	0	0.5	1.3	98.2	100
250 (B2G)--V	15.839	0	0.9	1.7	97.4	100
251 B2U)--V	15.856	0	1.3	0.1	98.6	100
252 (A2G)--V	15.892	0	0.3	0.9	98.8	100
253 (A1G)--V	15.923	1.6	1.4	12.4	84.6	100
254 (A2U)--V	15.951	9.4	1.5	1.4	87.7	100
255 (EU)--V	16.112	0.1	1	1.2	97.7	100
256 (EU)--V	16.112	0.1	1	1.2	97.7	100
257 (EG)--V	16.148	0	0.5	1.5	98	100
258 (EG)--V	16.148	0	0.5	1.5	98	100
259 (B1G)--V	16.201	0	24.7	1.2	74.1	100
260 (A1U)--V	16.288	0	0	0	100	100
261 (EU)--V	16.707	0.3	16.3	14.9	68.5	100
262 (EU)--V	16.707	0.3	16.3	14.9	68.5	100
263 (A1G)--V	16.726	1.1	0.4	9.1	89.5	100
264 (A2G)--V	16.885	0	0.8	1.1	98.1	100
265 (B1G)--V	16.904	0	0.4	1	98.6	100
266 (EU)--V	16.916	0.2	0.9	0.3	98.6	100
267 (EU)--V	16.916	0.2	0.9	0.3	98.6	100
268 (A1G)--V	16.969	0.9	23	7.7	68.4	100
269 (B2G)--V	16.972	0	0.7	7.8	91.4	100
270 (B1U)--V	17.105	0	0	1.1	98.9	100
271 (EU)--V	17.29	1.2	23.5	9.6	65.8	100
272 (EU)--V	17.29	1.2	23.5	9.6	65.8	100
273 (A1G)--V	17.3	0.4	13.7	23.3	62.5	100
274 (EG)--V	17.33	0	3.5	0.6	95.9	100
275 (EG)--V	17.33	0	3.5	0.6	95.9	100
276 A2G)--V	17.62	0	1	3.3	95.7	100
277 (EU)--V	17.958	1.9	3.3	1.4	93.4	100
278 (EU)--V	17.958	1.9	3.3	1.4	93.4	100
279 (EG)--V	18.05	0	1.1	3.4	95.5	100
280 (EG)--V	18.05	0	1.1	3.4	95.5	100
281 A2U)--V	18.066	2.8	1.1	1.3	94.8	100
282 (EU)--V	18.105	1.2	1.5	14.2	83.1	100
283 (EU)--V	18.105	1.2	1.5	14.2	83.1	100
284 (B2G)--V	18.159	0	0.6	14.4	85	100

285 (B2U)--V	18.19	0	1.6	0	98.4	100
286 A1U)--V	18.242	0	0	0	100	100
287 (B1G)--V	18.595	0.1	12.6	8.6	78.8	100
288 (B1U)--V	18.941	0	0	2.3	97.7	100
289 (EG)--V	19.065	0	0.5	0.3	99.2	100
290 (EG)--V	19.065	0	0.5	0.3	99.2	100
291 A2U)--V	19.257	0.6	0.4	3.4	95.6	100
292 (A1G)--V	19.479	5.8	22.1	4.2	68	100
293 (B2U)--V	20.5	0	1	0	99	100
294 (EG)--V	20.562	0	1.1	1.5	97.4	100
295 (EG)--V	20.562	0	1.1	1.5	97.4	100
296 A1U)--V	20.753	0	0	0	100	100
297 (EU)--V	20.822	5.4	14.7	7.4	72.5	100
298 (EU)--V	20.822	5.4	14.7	7.4	72.5	100
299 (B1U)--V	21.303	0	0	3.3	96.7	100
300 (EG)--V	21.848	0.2	33.5	6.4	59.9	100
301 (EG)--V	21.848	0.2	33.5	6.4	59.9	100
302 (B2G)--V	21.945	0	0.2	3.1	96.7	100
303 (EU)--V	22.133	0.1	1.1	1.6	97.2	100
304 (EU)--V	22.133	0.1	1.1	1.6	97.2	100
305 (A1G)--V	22.252	0.1	0.4	0.9	98.6	100
306 B2G)--V	22.627	0	1.8	1.5	96.7	100
307 (A2U)--V	22.686	1.1	11.9	57.4	29.5	100
308 (A2G)--V	22.844	0	0.3	1	98.7	100
309 (EU)--V	22.908	0.1	0	1.1	98.8	100
310 (EU)--V	22.908	0.1	0	1.1	98.8	100
311 (EG)--V	22.93	0	2.9	0.6	96.5	100
312 (EG)--V	22.93	0	2.9	0.6	96.5	100
313 (A2G)--V	23.206	0	1.6	1	97.4	100
314 (EU)--V	23.333	0	0.9	0.3	98.8	100
315 (EU)--V	23.333	0	0.9	0.3	98.8	100
316 B1G)--V	23.374	0	1	0.5	98.5	100
317 (B2G)--V	23.639	0	7.9	11.3	80.7	100
318 (A1G)--V	23.824	0.5	9.8	7.6	82.1	100
319 (B2G)--V	23.857	0	4.5	1.6	93.8	100
320 (EU)--V	23.963	0.2	2.1	3.7	94	100
321 (EU)--V	23.963	0.2	2.1	3.7	94	100
322 (A2G)--V	24.364	0	0.6	8.9	90.5	100
323 (A1U)--V	24.478	0	0	0	100	100
324 (B2U)--V	24.487	0	69.4	0	30.6	100
325 (B1G)--V	24.533	0	0.4	0	99.6	100
326 (EU)--V	24.536	0.1	0.8	3.4	95.7	100
327 (EU)--V	24.536	0.1	0.8	3.4	95.7	100
328 (A1G)--V	24.7	2.2	2.4	25.2	70.2	100
329 (EG)--V	25.206	0.1	14.4	42.1	43.4	100
330 (EG)--V	25.206	0.1	14.4	42.1	43.4	100
331 B1G)--V	25.216	0	20.1	10.9	68.9	100
332 (B1U)--V	25.28	0	0	64.2	35.8	100
333 (A1G)--V	25.372	0.8	10.3	6.4	82.5	100
334 (EU)--V	25.495	0.3	3.3	7	89.4	100
335 (EU)--V	25.495	0.3	3.3	7	89.4	100

336 (EU)--V	25.825	0.4	9.9	5.3	84.5	100
337 (EU)--V	25.825	0.4	9.9	5.3	84.5	100
338 (A2G)--V	25.979	0	0	0	100	100
339 (B1G)--V	26.138	0	0.3	0.3	99.5	100
340 (EU)--V	26.51	0.4	0.2	4.3	95.1	100
341 (EU)--V	26.51	0.4	0.2	4.3	95.1	100
342 (B2G)--V	27.064	0	0.1	0.9	99	100
343 (A2G)--V	27.256	0	0	1.7	98.3	100
344 (EU)--V	27.293	0.1	1.3	2.7	96	100
345 (EU)--V	27.293	0.1	1.3	2.7	96	100
346 A2U)--V	27.293	4.6	43.5	15.9	36	100
347 (B2G)--V	27.608	0	1	1.9	97.1	100
348 (B1G)--V	27.742	0	8	2.2	89.8	100
349 (EU)--V	27.927	0.4	6.2	3.4	90	100
350 (EU)--V	27.927	0.4	6.2	3.4	90	100
351 (EU)--V	28.356	0	5.6	5.7	88.7	100
352 (EU)--V	28.356	0	5.6	5.7	88.7	100
353 (A1G)--V	28.399	0	3.4	3.4	93.1	100
354 (A1G)--V	28.627	0.2	5.6	6.6	87.6	100
355 (B2G)--V	29.131	0	7.2	4	88.8	100
356 (EU)--V	29.577	0	2.4	3	94.7	100
357 (EU)--V	29.577	0	2.4	3	94.7	100
358 (A2G)--V	29.644	0	0.7	0.2	99	100
359 (A2G)--V	30.623	0	2.9	2.3	94.7	100
360 (B1G)--V	30.809	0	0.7	14.6	84.7	100
361 (EU)--V	30.876	0.1	1	0.7	98.2	100
362 (EU)--V	30.876	0.1	1	0.7	98.2	100
363 (B2G)--V	31.045	0	0.9	4.2	94.9	100
364 (B1G)--V	31.295	0	4.8	12.5	82.7	100
365 (A1G)--V	31.59	0.7	6.2	3.7	89.4	100
366 (EU)--V	31.686	0.1	5.6	3.4	90.9	100
367 (EU)--V	31.686	0.1	5.6	3.4	90.9	100
368 (B2G)--V	32.027	0	1.7	3.2	95.1	100
369 (A1G)--V	32.804	5.3	3.7	0.5	90.6	100
370 (EU)--V	33.014	1	6	4.7	88.2	100
371 (EU)--V	33.014	1	6	4.7	88.2	100
372 (B2U)--V	33.02	0	8.2	8.6	83.3	100
373 (A2G)--V	33.225	0	1.1	14.3	84.7	100
374 (EG)--V	33.422	0.1	5.7	14.5	79.7	100
375 (EG)--V	33.422	0.1	5.7	14.5	79.7	100
376 B1G)--V	34.057	0.4	14.3	8.4	77	100
377 (A2U)--V	34.07	0.2	0.9	10.9	88.1	100
378 (EU)--V	34.119	0.2	3.6	9.6	86.6	100
379 (EU)--V	34.119	0.2	3.6	9.6	86.6	100
380 (B2G)--V	34.409	0	1.7	1.9	96.4	100
381 A1U)--V	34.934	0	20	17.9	62.1	100
382 (EG)--V	34.982	0	8.6	9.5	81.9	100
383 (EG)--V	34.982	0	8.6	9.5	81.9	100
384 (B2U)--V	35.078	0	6.5	9.5	83.9	100
385 (EU)--V	35.171	0.2	1.7	12.5	85.7	100
386 (EU)--V	35.171	0.2	1.7	12.5	85.7	100

387 (A2G)--V	35.57	0	0.8	8.6	90.6	100
388 (B1U)--V	35.978	0	5.2	6.9	87.8	100
389 (B1G)--V	36.03	0	0.4	4.3	95.2	100
390 (EG)--V	36.079	0.2	5.3	7.5	87.1	100
391 (EG)--V	36.079	0.2	5.3	7.5	87.1	100
392 (A1U)--V	36.324	0	3.5	5.9	90.5	100
393 (A2U)--V	36.781	4.2	27.4	17.2	51.1	100
394 (A1G)--V	36.922	3.5	5.8	0.1	90.5	100
395 (EG)--V	36.939	1.9	18.6	7.9	71.6	100
396 (EG)--V	36.939	1.9	18.6	7.9	71.6	100
397 (B1G)--V	36.947	0	6	0.2	93.8	100
398 (EU)--V	36.948	0.1	3.7	0.6	95.6	100
399 (EU)--V	36.948	0.1	3.7	0.6	95.6	100
400 (EU)--V	37.751	0.3	6.7	0.2	92.8	100
401 (EU)--V	37.751	0.3	6.7	0.2	92.8	100
402 (B2U)--V	38.578	0	28.1	0.7	71.2	100
403 (A1G)--V	38.75	0.1	0.5	0	99.4	100
404 (EU)--V	39.005	0.1	1.1	1.6	97.2	100
405 (EU)--V	39.005	0.1	1.1	1.6	97.2	100
406 A2G)--V	39.008	0	3	17.6	79.5	100
407 (B2G)--V	39.014	0	0.1	0.4	99.5	100
408 (B1G)--V	39.071	0	0.1	1.2	98.7	100
409 (EG)--V	39.405	0.1	3.6	5.4	90.8	100
410 (EG)--V	39.405	0.1	3.6	5.4	90.8	100
411 A2U)--V	39.417	0.4	1.6	2.1	95.8	100
412 (B2U)--V	39.484	0	0.2	0.6	99.1	100
413 (EG)--V	39.734	0.5	13.5	12.8	73.3	100
414 (EG)--V	39.734	0.5	13.5	12.8	73.3	100
415 (A2U)--V	39.98	2.5	10.9	0.7	85.9	100
416 B1U)--V	40.333	0	18.9	24.4	56.7	100
417 (B2U)--V	40.361	0	2.2	0.7	97	100
418 (EG)--V	40.624	0.2	5.5	2.7	91.6	100
419 (EG)--V	40.624	0.2	5.5	2.7	91.6	100
420 (A1U)--V	40.659	0	0	0	100	100
421 (EU)--V	40.692	0	1.4	0.8	97.8	100
422 (EU)--V	40.692	0	1.4	0.8	97.8	100
423 (B1U)--V	40.716	0	3.7	5.1	91.2	100
424 (EG)--V	40.744	0.5	13.8	8	77.6	100
425 (EG)--V	40.744	0.5	13.8	8	77.6	100
426 A2G)--V	41.315	0	4.3	0	95.6	100
427 (A2U)--V	41.577	7.8	38.6	6.1	47.5	100
428 (A2G)--V	42.379	0	2.4	4.6	93	100
429 (B2G)--V	43.174	0	0.1	1.4	98.5	100
430 (EU)--V	43.218	0.2	4.6	0.2	95	100
431 (EU)--V	43.218	0.2	4.6	0.2	95	100
432 (A1G)--V	43.548	0.1	42.5	0.7	56.7	100
433 (EU)--V	43.775	0.8	14.1	2.7	82.4	100
434 (EU)--V	43.775	0.8	14.1	2.7	82.4	100
435 (A1G)--V	44.831	0.5	40.6	1.6	57.3	100
436 B1G)--V	45.24	0	35	2.9	62.1	100
437 (B2G)--V	46.185	0	0.2	20.5	79.4	100



438 (EU)--V	46.902	0.6	0.6	45	53.7	100
439 (EU)--V	46.902	0.6	0.6	45	53.7	100
440 (A1G)--V	47.169	1	1.2	54.4	43.3	100
441 B1G)--V	47.791	0	43.1	10.5	46.3	100
442 (B1U)--V	48.078	0	1.5	12.6	86	100
443 (EU)--V	48.079	0.2	33.6	4	62.2	100
444 (EU)--V	48.079	0.2	33.6	4	62.2	100
445 (A1G)--V	48.245	0.6	43.6	3.4	52.4	100
446 (EG)--V	48.403	0	2.5	10.2	87.3	100
447 (EG)--V	48.403	0	2.5	10.2	87.3	100
448 (A1U)--V	48.89	0	3.6	2.7	93.7	100
449 (B1G)--V	49.345	0	52.3	1.4	46.3	100
450 (B2G)--V	49.738	0	0.1	7.8	92.1	100
451 (EU)--V	49.893	0.1	18.6	3.8	77.5	100
452 (EU)--V	49.893	0.1	18.6	3.8	77.5	100
453 (A1G)--V	49.962	0.1	14.2	9.9	75.9	100
454 (EU)--V	50.05	0.1	1.6	20.4	77.9	100
455 (EU)--V	50.05	0.1	1.6	20.4	77.9	100
456 A2G)--V	50.215	0	0.5	0	99.5	100
457 (A2U)--V	50.257	0.5	10.6	25.2	63.7	100
458 (A1G)--V	50.669	0.5	20.3	37.7	41.5	100
459 (EU)--V	51.158	0	6.8	1	92.2	100
460 (EU)--V	51.158	0	6.8	1	92.2	100
461 B1G)--V	51.183	0	31.1	5.2	63.8	100
462 (EG)--V	51.362	0.4	16	17.5	66.1	100
463 (EG)--V	51.362	0.4	16	17.5	66.1	100
464 (A2G)--V	51.635	0	0.1	0	99.9	100
465 (B2G)--V	51.844	0	0	1.1	98.9	100
466 (EU)--V	51.951	0	0.6	1.1	98.3	100
467 (EU)--V	51.951	0	0.6	1.1	98.3	100
468 (A1G)--V	52.239	0	10.2	36.7	53.1	100
469 (B2U)--V	52.437	0	26.3	11.6	62.1	100
470 (EU)--V	52.558	1.7	5.8	18.2	74.2	100
471 (EU)--V	52.558	1.7	5.8	18.2	74.2	100
472 (B1G)--V	52.616	0	14.1	5.5	80.4	100
473 (B1G)--V	52.775	0	0.9	0.1	98.9	100
474 (EU)--V	53.057	2.4	13.5	9.6	74.6	100
475 (EU)--V	53.057	2.4	13.5	9.6	74.6	100
476 (EU)--V	53.666	15	31.1	0.5	53.4	100
477 (EU)--V	53.666	15	31.1	0.5	53.4	100
478 (A1G)--V	53.966	0.5	7.4	12.2	79.9	100
479 (A2G)--V	53.975	0	0	0.6	99.3	100
480 (B2G)--V	54.557	0	0.4	8.1	91.5	100
481 B2U)--V	54.676	0	26.9	14.4	58.7	100
482 (EU)--V	54.889	0	2.5	0.9	96.6	100
483 (EU)--V	54.889	0	2.5	0.9	96.6	100
484 (EU)--V	55.655	0.1	8.5	4.7	86.7	100
485 (EU)--V	55.655	0.1	8.5	4.7	86.7	100
486 A1G)--V	55.7	0.1	18.5	13.8	67.7	100
487 (EG)--V	55.923	0.9	28.2	17.6	53.3	100
488 (EG)--V	55.923	0.9	28.2	17.6	53.3	100

489 (B1G)--V	56.113	0	28.9	4.2	66.9	100
490 (A2G)--V	57.069	0	7.9	4.7	87.5	100
491 B1U)--V	57.079	0	2.4	28.9	68.7	100
492 (A1U)--V	57.157	0	24.8	11.1	64.2	100
493 (EG)--V	57.172	2.4	5.2	20.1	72.3	100
494 (EG)--V	57.172	2.4	5.2	20.1	72.3	100
495 (A2U)--V	57.176	0.3	4.9	20.7	74.1	100
496 B2G)--V	57.361	0	0.2	0.1	99.7	100
497 (EU)--V	57.662	0.1	0.7	1.3	97.8	100
498 (EU)--V	57.662	0.1	0.7	1.3	97.8	100
499 (A2G)--V	57.891	0	2.2	2.3	95.4	100
500 (EU)--V	57.925	0	2.2	4.2	93.5	100
501 (EU)--V	57.925	0	2.2	4.2	93.5	100
502 (B1G)--V	58.514	0	4.3	8.9	86.8	100
503 (B2G)--V	58.599	0	0.4	6.6	93	100
504 (EU)--V	58.892	0.1	0.8	3.4	95.7	100
505 (EU)--V	58.892	0.1	0.8	3.4	95.7	100
506 A1G)--V	59.181	0.8	4.7	0.8	93.7	100
507 (EG)--V	59.423	17	13.7	2.2	67.1	100
508 (EG)--V	59.423	17	13.7	2.2	67.1	100
509 (B1U)--V	59.744	0	9.8	13.2	77	100
510 (EG)--V	60.242	62.4	9.3	2.7	25.6	100
511 (EG)--V	60.242	62.4	9.3	2.7	25.6	100
512 (A1U)--V	60.633	0	5.7	5	89.3	100
513 (B2U)--V	60.76	0	1	0	99	100
514 (A2G)--V	60.793	0	0	0.6	99.4	100
515 (EU)--V	61.034	0.1	4.3	7.7	87.9	100
516 (EU)--V	61.034	0.1	4.3	7.7	87.9	100
517 (EG)--V	61.328	0.4	9.1	0.1	90.5	100
518 (EG)--V	61.328	0.4	9.1	0.1	90.5	100
519 (B1U)--V	61.436	0	6.6	1.5	92	100
520 (EG)--V	61.638	3.5	1.7	6.5	88.2	100
521 (EG)--V	61.638	3.5	1.7	6.5	88.2	100
522 (A2U)--V	61.691	0.3	33.6	5.6	60.5	100
523 (A2U)--V	61.81	0.1	8.4	1.3	90.2	100
524 (A1U)--V	61.937	0	0.2	4.9	94.9	100
525 (B2G)--V	62.063	0	0.2	11.7	88.2	100
526 A2G)--V	62.168	0	4.3	1.7	94	100
527 (EU)--V	62.582	2.2	13.7	15.3	68.8	100
528 (EU)--V	62.582	2.2	13.7	15.3	68.8	100
529 (B1G)--V	62.766	0	35.8	16.6	47.5	100
530 (B2U)--V	62.839	0	2.4	1.2	96.4	100
531 (EG)--V	62.857	0	8.3	4.6	87.1	100
532 (EG)--V	62.857	0	8.3	4.6	87.1	100
533 (A1G)--V	63.618	0.1	1.3	17.6	81	100
534 (B2G)--V	64.575	5.7	3.9	8	82.5	100
535 (B1U)--V	64.695	0	18.2	1.7	80.2	100
536 (EU)--V	65.028	0.1	2	26.6	71.3	100
537 (EU)--V	65.028	0.1	2	26.6	71.3	100
538 (A2G)--V	65.692	0	0.1	0	99.9	100
539 (EG)--V	65.743	0.8	15.5	8.5	75.1	100

540 (EG)--V	65.743	0.8	15.5	8.5	75.1	100
541 (EU)--V	66.079	0	0.2	0.5	99.3	100
542 (EU)--V	66.079	0	0.2	0.5	99.3	100
543 (B2G)--V	66.316	0	2.1	23.9	74	100
544 (B1G)--V	66.413	0	1.9	0	98	100
545 (B2G)--V	67.066	0.7	5.8	9.8	83.7	100
546 A1U)--V	67.938	0	2.7	6.6	90.7	100
547 (A2U)--V	68.094	0.1	8.9	18.9	72.1	100
548 (A1G)--V	68.135	1.8	16	1	81.2	100
549 (EU)--V	68.302	0.2	8.4	11.6	79.8	100
550 (EU)--V	68.302	0.2	8.4	11.6	79.8	100
551 (EG)--V	69.163	0	7.6	9.9	82.5	100
552 (EG)--V	69.163	0	7.6	9.9	82.5	100
553 (A1U)--V	70.27	0	13.4	12.4	74.1	100
554 (B1U)--V	70.374	0	12.3	8.3	79.4	100
555 (A1G)--V	71.563	2.5	19.1	34.5	43.9	100
556 B1G)--V	71.658	0.6	57.5	4.5	37.4	100
557 (A2G)--V	71.779	0	0.6	0.2	99.2	100
558 (EU)--V	72.14	0	0.2	0.4	99.4	100
559 (EU)--V	72.14	0	0.2	0.4	99.4	100
560 (EG)--V	72.203	0.4	7.1	10.7	81.8	100
561 (EG)--V	72.203	0.4	7.1	10.7	81.8	100
562 (B2G)--V	72.214	0	0.3	0.1	99.6	100
563 (EU)--V	72.499	0.1	16.7	9.6	73.6	100
564 (EU)--V	72.499	0.1	16.7	9.6	73.6	100
565 (B1G)--V	72.716	0	1	2.1	96.8	100
566 (EU)--V	73.004	0.1	27.3	26.6	46.1	100
567 (EU)--V	73.004	0.1	27.3	26.6	46.1	100
568 (A1G)--V	73.048	1.6	14.3	26.3	57.7	100
569 (B1U)--V	73.052	0	0.1	4.1	95.7	100
570 (A2G)--V	73.136	0	2.9	2.1	95	100
571 (EU)--V	73.228	0.1	12.3	10.1	77.6	100
572 (EU)--V	73.228	0.1	12.3	10.1	77.6	100
573 (B1G)--V	73.376	0	27.3	5.3	67.3	100
574 (A1G)--V	74.094	6.5	11.4	4.7	77.4	100
575 (B2U)--V	74.188	0	15.9	30.8	53.3	100
576 A1U)--V	74.336	0	5.5	16.8	77.7	100
577 (EG)--V	74.39	0.2	9.9	22.2	67.6	100
578 (EG)--V	74.39	0.2	9.9	22.2	67.6	100
579 (B1G)--V	74.436	0.2	30.5	4.3	65.1	100
580 (EU)--V	74.474	0.1	42.7	13.1	44.1	100
581 (EU)--V	74.474	0.1	42.7	13.1	44.1	100
582 (A1G)--V	74.764	0.6	56.1	17.2	26.1	100
583 (B2G)--V	75.469	0	0.2	6.5	93.3	100
584 (B2G)--V	75.904	0.1	4.1	20	75.8	100
585 (EU)--V	76.176	0	1.8	6.2	92	100
586 (EU)--V	76.176	0	1.8	6.2	92	100
587 (A2G)--V	76.575	0	0.7	6.4	93	100
588 (B1G)--V	76.846	1.6	49.4	4.1	44.8	100
589 (B2G)--V	77.124	0	0.1	0.3	99.5	100
590 (EU)--V	77.825	0	3.1	4.6	92.2	100

591 (EU)--V	77.825	0	3.1	4.6	92.2	100
592 (EU)--V	79.282	0.1	7.3	4.4	88.1	100
593 (EU)--V	79.282	0.1	7.3	4.4	88.1	100
594 (A2G)--V	79.479	0	1.2	2.4	96.4	100
595 (A1G)--V	79.722	0.3	21.2	25.4	53.2	100
596 (EU)--V	79.937	0.3	5.9	6.4	87.3	100
597 (EU)--V	79.937	0.3	5.9	6.4	87.3	100
598 (B2G)--V	81.331	0	0.1	8.2	91.7	100
599 (B1G)--V	81.762	0.9	7.1	6.4	85.6	100
600 (A2G)--V	82.306	0	0.3	0.1	99.7	100
601 (EU)--V	82.986	0.1	10.1	10.9	78.9	100
602 (EU)--V	82.986	0.1	10.1	10.9	78.9	100
603 (A1G)--V	83.041	0.6	4.1	5.8	89.5	100
604 (A2G)--V	83.771	0	17.3	5	77.6	100
605 (B2G)--V	84.982	0	2.3	2.6	95.1	100
606 (EU)--V	85.47	0	1.1	5.5	93.4	100
607 (EU)--V	85.47	0	1.1	5.5	93.4	100
608 (EU)--V	87.873	0.2	7.2	19.9	72.8	100
609 (EU)--V	87.873	0.2	7.2	19.9	72.8	100
610 (B1G)--V	89.336	1	5.3	26.1	67.6	100
611 A1G)--V	91.192	0.4	3.9	55.3	40.3	100
612 (B2G)--V	91.601	0	1	1.9	97	100
613 (EU)--V	92.805	0	1.5	3.1	95.4	100
614 (EU)--V	92.805	0	1.5	3.1	95.4	100
615 (A2G)--V	93.491	0	8.1	13.3	78.6	100
616 A2G)--V	93.613	0	1.1	0.7	98.1	100
617 (EU)--V	95.529	0	5.6	4.5	89.9	100
618 (EU)--V	95.529	0	5.6	4.5	89.9	100
619 (B2G)--V	96.204	0	4	3.1	92.9	100

## BHandH Exchange Correlation Functional

Orbital	Index	E, eV	Zn	NZn	Nmeso	Pc	Total	
	1 A1G)--O	-9500.28		100	0	0	0	100
	2 (A1G)--O	-1169.44		100	0	0	0	100
	3 (A2U)--O	-1029.32		100	0	0	0	100
	4 (EU)--O	-1029.15		100	0	0	0	100
	5 (EU)--O	-1029.15		100	0	0	0	100
	6 B1G)--O	-400.956		0	99.9	0	0.1	100
	7 (EU)--O	-400.956		0	99.9	0	0.1	100
	8 (EU)--O	-400.956		0	99.9	0	0.1	100
	9 (A1G)--O	-400.955		0	99.9	0	0.1	100
	10 (B2G)--O	-400.72		0	0	99.8	0.2	100
	11 (EU)--O	-400.72		0	0	99.8	0.1	100
	12 (EU)--O	-400.72		0	0	99.8	0.1	100
	13 (A1G)--O	-400.72		0	0	99.9	0.1	100
	14 (B2G)--O	-288.156		0	0	0.1	99.9	100
	15 (EU)--O	-288.156		0	0	0.1	99.9	100
	16 (EU)--O	-288.156		0	0	0.1	99.9	100

17 (A1G)--O	-288.155	0	0	0	100	100
18 (A2G)--O	-288.155	0	0	0	100	100
19 (EU)--O	-288.155	0	0	0	100	100
20 (EU)--O	-288.155	0	0	0	100	100
21 B1G)--O	-288.155	0	0	0	100	100
22 (EU)--O	-286.187	0	0	0	100	100
23 (EU)--O	-286.187	0	0	0	100	100
24 (A1G)--O	-286.187	0	0	0	100	100
25 (B1G)--O	-286.187	0	0	0	100	100
26 A2G)--O	-286.171	0	0	0	100	100
27 (EU)--O	-286.171	0	0	0	100	100
28 (EU)--O	-286.171	0	0	0	100	100
29 (B2G)--O	-286.171	0	0	0	100	100
30 (B1G)--O	-286.142	0	0	0	100	100
31 (EU)--O	-286.142	0	0	0	100	100
32 (EU)--O	-286.142	0	0	0	100	100
33 (A1G)--O	-286.142	0	0	0	100	100
34 (A2G)--O	-286.14	0	0	0	100	100
35 (EU)--O	-286.14	0	0	0	100	100
36 (EU)--O	-286.14	0	0	0	100	100
37 (B2G)--O	-286.14	0	0	0	100	100
38 (B1G)--O	-286.112	0	0	0	100	100
39 (EU)--O	-286.112	0	0	0	100	100
40 (EU)--O	-286.112	0	0	0	100	100
41 A1G)--O	-286.112	0	0	0	100	100
42 (A2G)--O	-286.096	0	0	0	100	100
43 (EU)--O	-286.096	0	0	0	100	100
44 (EU)--O	-286.096	0	0	0	100	100
45 (B2G)--O	-286.096	0	0	0	100	100
46 A1G)--O	-138.877	100	0	0	0	100
47 (A2U)--O	-93.523	100	0	0	0	100
48 (EU)--O	-93.311	100	0	0	0	100
49 (EU)--O	-93.311	100	0	0	0	100
50 (A1G)--O	-30.935	0.4	39.8	25.6	34.2	100
51 (EU)--O	-30.503	0.2	38.7	25.5	35.6	100
52 (EU)--O	-30.503	0.2	38.7	25.5	35.6	100
53 (B1G)--O	-29.649	0.2	59.5	0.8	39.5	100
54 (B2G)--O	-29.045	0	1.7	70.1	28.2	100
55 (EU)--O	-27.793	0.1	18.1	50	31.9	100
56 (EU)--O	-27.793	0.1	18.1	50	31.9	100
57 (A1G)--O	-26.852	0.1	15.6	49	35.3	100
58 (A1G)--O	-26.39	0.4	24.4	10.4	64.8	100
59 (EU)--O	-26.375	0.1	15.5	1.3	83.1	100
60 (EU)--O	-26.375	0.1	15.5	1.3	83.1	100
61 B1G)--O	-26.359	0.1	13.9	0	86	100
62 (A2G)--O	-23.954	0	2.7	6.4	90.8	100
63 (A1G)--O	-23.61	0.7	12.4	0.3	86.6	100
64 (EU)--O	-23.567	0.1	14.7	3.5	81.7	100
65 (EU)--O	-23.567	0.1	14.7	3.5	81.7	100
66 B1G)--O	-23.439	0.7	19.2	0.5	79.5	100
67 (EU)--O	-23.438	0	3.5	1.6	94.8	100

68 (EU)--O	-23.438	0	3.5	1.6	94.8	100
69 (B2G)--O	-23.342	0	0	1.8	98.2	100
70 (A2G)--O	-22.311	0	6.2	9.7	84	100
71 (EU)--O	-21.506	0	7.8	19.5	72.7	100
72 (EU)--O	-21.506	0	7.8	19.5	72.7	100
73 (B1G)--O	-19.905	2.5	13.3	17.8	66.5	100
74 (A1G)--O	-19.785	2.6	12	0.3	85.1	100
75 (EU)--O	-19.58	0.2	10.7	0.3	88.8	100
76 (EU)--O	-19.58	0.2	10.7	0.3	88.8	100
77 (B2G)--O	-19.441	0.1	3.4	12.7	83.7	100
78 (B1G)--O	-19.263	1.5	3.7	13.7	81	100
79 (EU)--O	-18.538	0	6.4	4.2	89.4	100
80 (EU)--O	-18.538	0	6.4	4.2	89.4	100
81 B2G)--O	-18.492	4.6	31.4	21.3	42.7	100
82 (A2G)--O	-18.243	0	7.1	2.2	90.6	100
83 (A1G)--O	-17.354	8.7	11.3	1.3	78.6	100
84 (EU)--O	-17.107	0	19.8	13.1	67.1	100
85 (EU)--O	-17.107	0	19.8	13.1	67.1	100
86 B1G)--O	-17.002	48.8	16.4	2.8	32	100
87 (EU)--O	-16.64	0.3	15.9	20	63.7	100
88 (EU)--O	-16.64	0.3	15.9	20	63.7	100
89 (B1G)--O	-15.964	40.9	4.3	2.6	52.3	100
90 (A1G)--O	-15.926	70.3	10.9	0.7	18.1	100
91 B2G)--O	-15.778	16.8	2.8	1.2	79.2	100
92 (EG)--O	-15.736	95	3.8	0.3	0.9	100
93 (EG)--O	-15.736	95	3.8	0.3	0.9	100
94 (A2G)--O	-15.636	0	29.2	16.8	54	100
95 (B2G)--O	-15.088	58.4	4.6	1.6	35.4	100
96 (EU)--O	-15.077	0	3.2	5.1	91.8	100
97 (EU)--O	-15.077	0	3.2	5.1	91.8	100
98 (A1G)--O	-14.712	32.3	7.4	2.2	58.2	100
99 (EU)--O	-14.622	0.6	13.2	1.1	85.2	100
100 (EU)--O	-14.622	0.6	13.2	1.1	85.2	100
101 A2U)--O	-14.511	0.4	27.5	18.8	53.3	100
102 (A2G)--O	-14.48	0	0.7	8.9	90.4	100
103 (B1G)--O	-14.331	7.4	7.3	1	84.3	100
104 (A1G)--O	-13.95	3.5	4.4	4	88.2	100
105 (EG)--O	-13.894	10	19.8	16.4	53.9	100
106 (EG)--O	-13.894	10	19.8	16.4	53.9	100
107 (EU)--O	-13.789	0.1	1.8	1.8	96.3	100
108 (EU)--O	-13.789	0.1	1.8	1.8	96.3	100
109 (B2G)--O	-13.759	0.1	0	1.2	98.7	100
110 (A2G)--O	-13.467	0	0.5	3.7	95.7	100
111 (EU)--O	-13.413	0.3	6.5	4.5	88.7	100
112 (EU)--O	-13.413	0.3	6.5	4.5	88.7	100
113 (B1G)--O	-13.128	4.9	2.2	4.5	88.3	100
114 (B2U)--O	-13.1	0	29.1	0	70.8	100
115 (A1G)--O	-12.722	24.2	24.2	6.8	44.8	100
116 B1U)--O	-12.046	0	0	52.9	47	100
117 (B2G)--O	-11.747	0.1	0	2.1	97.7	100
118 (EU)--O	-11.67	0.2	4	4.1	91.7	100

119 (EU)--O	-11.67	0.2	4	4.1	91.7	100
120 (EG)--O	-11.455	0.4	3.5	12.8	83.3	100
121 (EG)--O	-11.455	0.4	3.5	12.8	83.3	100
122 (A2U)--O	-11.438	0.3	8.2	3.5	88.1	100
123 (A2G)--O	-11.436	0	1.9	1.1	97	100
124 (EU)--O	-11.395	3.9	39.4	3.8	52.8	100
125 (EU)--O	-11.395	3.9	39.4	3.8	52.8	100
126 A1G)--O	-11.23	0	2.2	4.1	93.7	100
127 (B2U)--O	-10.956	0	29.4	0	70.6	100
128 (EU)--O	-10.881	1	9.6	6.6	82.7	100
129 (EU)--O	-10.881	1	9.6	6.6	82.7	100
130 (B1G)--O	-10.87	1.1	2	2.7	94.2	100
131 A1G)--O	-10.127	0.3	17	54.2	28.5	100
132 (EG)--O	-10.019	1	24.7	23.8	50.4	100
133 (EG)--O	-10.019	1	24.7	23.8	50.4	100
134 (EU)--O	-9.279	0.3	19.3	49.4	31	100
135 (EU)--O	-9.279	0.3	19.3	49.4	31	100
136 B2G)--O	-8.766	0.4	13.1	61.6	24.9	100
137 (A1U)--O	-8.639	0	0	0	100	100
138 (B1G)--O	-8.429	15.8	58.5	1	24.6	100
139 (A2U)--O	-8.224	2.3	46.2	20.4	31.1	100
140 (B1U)--O	-8.056	0	0	5	95	100
141 (EG)--O	-8.015	0	1.1	10	88.9	100
142 (EG)--O	-8.015	0	1.1	10	88.9	100
143 (EG)--O	-7.848	0.8	26.2	0.9	72.1	100
144 (EG)--O	-7.848	0.8	26.2	0.9	72.1	100
145 (B2U)--O	-7.794	0	24.3	0	75.7	100
146 A2U)--O	-7.766	0.2	6.6	39.4	53.7	100
147 (A1U)--O	-5.311	0	0.1	0.1	99.8	100
148 (EG)--V	-2.035	0.2	13.2	18.1	68.5	100
149 (EG)--V	-2.035	0.2	13.2	18.1	68.5	100
150 (B1U)--V	0.044	0	0	21.9	78.1	100
151 B2U)--V	0.331	0	18.2	0	81.8	100
152 (A2U)--V	0.431	14.6	0.2	5.8	79.4	100
153 (EG)--V	0.681	0.1	4.8	3.4	91.7	100
154 (EG)--V	0.681	0.1	4.8	3.4	91.7	100
155 (A2U)--V	1.706	62.9	9.4	0.3	27.5	100
156 A1G)--V	1.865	81.6	10.3	0.1	8	100
157 (A1U)--V	2.09	0	0	0	100	100
158 (EG)--V	2.182	0	1.8	1.1	97.1	100
159 (EG)--V	2.182	0	1.8	1.1	97.1	100
160 (B2U)--V	2.932	0	19.4	0.1	80.5	100
161 B1U)--V	3.252	0	0.1	20	80	100
162 (EU)--V	3.399	78.3	5.8	1.6	14.3	100
163 (EU)--V	3.399	78.3	5.8	1.6	14.3	100
164 (A1G)--V	3.931	0.3	0	1.4	98.3	100
165 (EU)--V	4.055	2.1	0.1	0.2	97.6	100
166 (EU)--V	4.055	2.1	0.1	0.2	97.6	100
167 (B1G)--V	4.149	0	0	0.1	99.9	100
168 (EG)--V	4.874	0.1	14.1	16	69.8	100
169 (EG)--V	4.874	0.1	14.1	16	69.8	100

170 (B2G)--V	4.96	0	0.7	0.1	99.2	100
171 A2U)--V	5.088	45.6	9.4	13.5	31.6	100
172 (EU)--V	5.205	0	0.9	0.3	98.7	100
173 (EU)--V	5.205	0	0.9	0.3	98.7	100
174 (A1G)--V	5.381	17.2	0.4	10.2	72.3	100
175 (A2G)--V	5.518	0	0.6	0.1	99.3	100
176 (EU)--V	5.891	0.5	0.1	2.9	96.5	100
177 (EU)--V	5.891	0.5	0.1	2.9	96.5	100
178 (B2G)--V	5.92	0	0	4.6	95.4	100
179 (A1G)--V	6.288	35.2	1.6	0.7	62.4	100
180 (EU)--V	6.39	0.3	1.4	0.1	98.2	100
181 (EU)--V	6.39	0.3	1.4	0.1	98.2	100
182 (B1G)--V	6.393	0	3	0.1	96.9	100
183 (A2G)--V	6.539	0	0	0.1	99.9	100
184 (A1U)--V	6.77	0	0	0	100	100
185 (B1U)--V	6.953	0	0	4.5	95.5	100
186 (EG)--V	6.966	0	0.9	4.2	94.9	100
187 (EG)--V	6.966	0	0.9	4.2	94.9	100
188 (B2G)--V	7.285	0.1	2.2	17.9	79.9	100
189 (EU)--V	7.34	4.1	9.7	6.2	80.1	100
190 (EU)--V	7.34	4.1	9.7	6.2	80.1	100
191 A1G)--V	7.743	0.3	0.9	2.7	96.2	100
192 (B1G)--V	7.952	0	31.9	2.5	65.6	100
193 (A2U)--V	8.173	72.5	7	3.9	16.6	100
194 (A2G)--V	8.33	0	5.3	0.4	94.2	100
195 (EU)--V	8.347	0.2	0.8	0.8	98.3	100
196 (EU)--V	8.347	0.2	0.8	0.8	98.3	100
197 (B2G)--V	8.606	0	0.4	9.8	89.7	100
198 (EU)--V	8.627	0.5	0.5	5.8	93.2	100
199 (EU)--V	8.627	0.5	0.5	5.8	93.2	100
200 (A2G)--V	8.842	0	0	0	100	100
201 B1G)--V	8.988	0	0.8	0	99.2	100
202 (EU)--V	9.297	0.9	2.7	1.6	94.8	100
203 (EU)--V	9.297	0.9	2.7	1.6	94.8	100
204 (A1G)--V	9.457	4	6	18.7	71.3	100
205 (A1G)--V	9.791	6.4	0.9	7.3	85.4	100
206 (EU)--V	9.879	0.7	11	3.7	84.6	100
207 (EU)--V	9.879	0.7	11	3.7	84.6	100
208 (B1G)--V	10.456	0	0.5	0.2	99.3	100
209 (B2G)--V	10.685	0	0.9	2.4	96.7	100
210 (EU)--V	10.768	0.3	4	16.7	79	100
211 (EU)--V	10.768	0.3	4	16.7	79	100
212 (A1G)--V	10.981	0.2	4	3.4	92.3	100
213 (EU)--V	11.107	1.7	3.5	0.2	94.6	100
214 (EU)--V	11.107	1.7	3.5	0.2	94.6	100
215 (B2G)--V	11.18	0	3.4	26	70.7	100
216 B1G)--V	11.646	0	5.8	0	94.1	100
217 (B2G)--V	12.028	0	3.6	7.9	88.4	100
218 (A1G)--V	12.232	1.2	19.3	11.2	68.3	100
219 (EU)--V	12.234	2.2	3.8	15.6	78.4	100
220 (EU)--V	12.234	2.2	3.8	15.6	78.4	100



221 A2G)--V	12.886	0	6.3	8.8	84.9	100
222 (B1G)--V	13.174	0	19.3	9.6	71.1	100
223 (EU)--V	13.407	2	9.7	10.7	77.6	100
224 (EU)--V	13.407	2	9.7	10.7	77.6	100
225 (A2G)--V	13.615	0	0.1	1.2	98.7	100
226 (EU)--V	13.807	0.8	1.3	3.1	94.9	100
227 (EU)--V	13.807	0.8	1.3	3.1	94.9	100
228 (EU)--V	15.542	2.1	3.3	3.5	91	100
229 (EU)--V	15.542	2.1	3.3	3.5	91	100
230 (EG)--V	15.689	0	1.4	1.3	97.3	100
231 (EG)--V	15.689	0	1.4	1.3	97.3	100
232 (A2G)--V	15.924	0	0.2	5.4	94.4	100
233 (B2U)--V	15.934	0	0.4	0	99.5	100
234 (A2U)--V	16.047	3.7	0.2	0.6	95.4	100
235 (B2G)--V	16.127	0	0.4	0	99.6	100
236 B1G)--V	16.475	0	33.8	5.1	61.1	100
237 (A1G)--V	16.498	0.6	4	1.4	94	100
238 (EG)--V	16.604	0	1.7	1.5	96.8	100
239 (EG)--V	16.604	0	1.7	1.5	96.8	100
240 (EU)--V	16.79	0.1	1.1	3	95.7	100
241 (EU)--V	16.79	0.1	1.1	3	95.7	100
242 (B1U)--V	16.865	0	0	3.9	96.1	100
243 (A2G)--V	16.957	0	1.3	4.5	94.2	100
244 (EU)--V	17.035	0.5	0.7	2.9	96	100
245 (EU)--V	17.035	0.5	0.7	2.9	96	100
246 B1G)--V	17.144	0	4.5	0.9	94.5	100
247 (B2G)--V	17.327	0	0.6	1.9	97.5	100
248 (B2U)--V	17.44	0	1.3	0.1	98.6	100
249 (A2U)--V	17.508	8.8	1.5	1.3	88.4	100
250 (EU)--V	17.571	0.1	0.3	0.5	99.2	100
251 (EU)--V	17.571	0.1	0.3	0.5	99.2	100
252 (A1G)--V	17.747	1.9	0.3	10.4	87.4	100
253 (EG)--V	17.753	0	0.5	1.5	98.1	100
254 (EG)--V	17.753	0	0.5	1.5	98.1	100
255 (A1U)--V	17.898	0	0	0	100	100
256 B2G)--V	17.904	0	1	1.4	97.7	100
257 (A2G)--V	17.929	0	0.2	0.5	99.3	100
258 (EU)--V	17.966	0.2	0.9	0.7	98.3	100
259 (EU)--V	17.966	0.2	0.9	0.7	98.3	100
260 (B1G)--V	18.034	0	23.8	0.9	75.3	100
261 A1G)--V	18.443	0.9	22.1	6.1	70.9	100
262 (EU)--V	18.589	0.5	21.7	11.5	66.4	100
263 (EU)--V	18.589	0.5	21.7	11.5	66.4	100
264 (A1G)--V	18.662	0.3	12.7	20.5	66.5	100
265 (B1U)--V	18.739	0	0	1	99	100
266 A2G)--V	18.855	0	0.6	1.1	98.3	100
267 (B2G)--V	18.871	0	0.8	5	94.2	100
268 (B1G)--V	18.88	0	2	1.6	96.5	100
269 (EU)--V	18.887	0.1	0.9	1.5	97.5	100
270 (EU)--V	18.887	0.1	0.9	1.5	97.5	100
271 (EG)--V	18.997	0	3	0.6	96.4	100

272 (EG)--V	18.997	0	3	0.6	96.4	100
273 (EU)--V	19.013	1.3	21.7	6.5	70.4	100
274 (EU)--V	19.013	1.3	21.7	6.5	70.4	100
275 (A1G)--V	19.355	1.4	3.7	22.9	72.1	100
276 A2G)--V	19.755	0	1.1	3.6	95.3	100
277 (A2U)--V	19.76	2.6	1	1.2	95.1	100
278 (EG)--V	19.79	0	1	3.1	95.9	100
279 (EG)--V	19.79	0	1	3.1	95.9	100
280 (B2U)--V	19.934	0	1.4	0	98.6	100
281 A1U)--V	19.958	0	0	0	100	100
282 (EU)--V	19.981	1.8	3.8	1.8	92.5	100
283 (EU)--V	19.981	1.8	3.8	1.8	92.5	100
284 (EU)--V	20.337	0.9	1.3	14.8	83	100
285 (EU)--V	20.337	0.9	1.3	14.8	83	100
286 B2G)--V	20.383	0	0.5	14	85.5	100
287 (B1U)--V	20.702	0	0	2.3	97.7	100
288 (EG)--V	20.82	0	0.4	0.3	99.3	100
289 (EG)--V	20.82	0	0.4	0.3	99.3	100
290 (A2U)--V	20.99	0.5	0.4	2.9	96.3	100
291 B1G)--V	21.04	0.1	9.6	10.6	79.7	100
292 (A1G)--V	21.415	5.3	21.9	4.1	68.7	100
293 (B2U)--V	22.211	0	0.9	0	99.1	100
294 (EG)--V	22.318	0	0.6	1.1	98.3	100
295 (EG)--V	22.318	0	0.6	1.1	98.3	100
296 A1U)--V	22.484	0	0	0	100	100
297 (EU)--V	22.717	5	13.7	6.7	74.5	100
298 (EU)--V	22.717	5	13.7	6.7	74.5	100
299 (B1U)--V	23.115	0	0	3.1	96.9	100
300 (EG)--V	23.77	0.2	27.8	6	66	100
301 (EG)--V	23.77	0.2	27.8	6	66	100
302 (B2G)--V	24.235	0	0.6	3.2	96.2	100
303 (EU)--V	24.379	0.1	1.5	1.8	96.6	100
304 (EU)--V	24.379	0.1	1.5	1.8	96.6	100
305 (A1G)--V	24.485	0.1	0.6	1.4	97.9	100
306 A2U)--V	24.689	1.1	11.6	59.4	28	100
307 (EG)--V	24.788	0	4.7	1	94.3	100
308 (EG)--V	24.788	0	4.7	1	94.3	100
309 (B2G)--V	24.816	0	2.3	2	95.7	100
310 (A2G)--V	25.053	0	0.6	1.3	98.1	100
311 (EU)--V	25.159	0.1	0	1	98.9	100
312 (EU)--V	25.159	0.1	0	1	98.9	100
313 (A2G)--V	25.374	0	2	1.1	96.8	100
314 (EU)--V	25.613	0	1.2	0.3	98.4	100
315 (EU)--V	25.613	0	1.2	0.3	98.4	100
316 B1G)--V	25.676	0	2	1.1	96.9	100
317 (B2G)--V	25.727	0	1.3	12.9	85.8	100
318 (A1G)--V	25.756	0.5	10.3	7.5	81.7	100
319 (EU)--V	25.925	0.1	2.9	4.2	92.8	100
320 (EU)--V	25.925	0.1	2.9	4.2	92.8	100
321 B2G)--V	26.018	0	8.1	2.7	89.3	100
322 (A1U)--V	26.28	0	0	0	100	100

323 (A2G)--V	26.51	0	0.2	6.7	93.1	100
324 (EU)--V	26.603	0.1	1.4	4	94.5	100
325 (EU)--V	26.603	0.1	1.4	4	94.5	100
326 B1G)--V	26.615	0	0.3	0.4	99.3	100
327 (B2U)--V	26.621	0	70.8	0	29.2	100
328 (A1G)--V	26.676	2.4	2.6	25.4	69.7	100
329 (B1G)--V	27.222	0	20.1	11.9	68	100
330 (EG)--V	27.223	0.1	15	42.3	42.6	100
331 (EG)--V	27.223	0.1	15	42.3	42.6	100
332 (B1U)--V	27.267	0	0	65.4	34.6	100
333 (A1G)--V	27.388	0.7	9.3	5.3	84.7	100
334 (EU)--V	27.566	0.1	3.9	6.1	89.8	100
335 (EU)--V	27.566	0.1	3.9	6.1	89.8	100
336 (EU)--V	27.8	0.6	10.2	5.6	83.7	100
337 (EU)--V	27.8	0.6	10.2	5.6	83.7	100
338 (A2G)--V	28.019	0	0	0	100	100
339 (B1G)--V	28.058	0	0.3	0.2	99.5	100
340 (EU)--V	28.497	0.4	0.2	4.9	94.5	100
341 (EU)--V	28.497	0.4	0.2	4.9	94.5	100
342 (B2G)--V	29.103	0	0.4	1.3	98.3	100
343 (EU)--V	29.34	0.1	2.1	3.1	94.6	100
344 (EU)--V	29.34	0.1	2.1	3.1	94.6	100
345 (A2U)--V	29.415	4.6	44.2	15.8	35.3	100
346 A2G)--V	29.448	0	0	1.8	98.2	100
347 (B2G)--V	29.596	0	0.7	1.5	97.8	100
348 (B1G)--V	29.639	0	7.7	2.6	89.7	100
349 (EU)--V	29.918	0.2	5.1	3	91.7	100
350 (EU)--V	29.918	0.2	5.1	3	91.7	100
351 (EU)--V	30.281	0	4.8	5.5	89.7	100
352 (EU)--V	30.281	0	4.8	5.5	89.7	100
353 (A1G)--V	30.365	0	3.8	3.5	92.6	100
354 (A1G)--V	30.613	0.2	5.2	7.1	87.6	100
355 (B2G)--V	30.958	0	7	4.1	88.9	100
356 (EU)--V	31.547	0	2.9	3.4	93.7	100
357 (EU)--V	31.547	0	2.9	3.4	93.7	100
358 (A2G)--V	31.574	0	0.7	0.3	99	100
359 (A2G)--V	32.657	0	3.5	3.6	92.9	100
360 (B1G)--V	32.884	0	1.4	16.2	82.5	100
361 (EU)--V	32.961	0.1	0.8	1.1	98.1	100
362 (EU)--V	32.961	0.1	0.8	1.1	98.1	100
363 (B2G)--V	33.203	0	0.9	4	95.1	100
364 (B1G)--V	33.306	0	4.9	10.5	84.6	100
365 (A1G)--V	33.691	0.7	5.9	3.7	89.7	100
366 (EU)--V	33.809	0.1	5.5	4	90.3	100
367 (EU)--V	33.809	0.1	5.5	4	90.3	100
368 (B2G)--V	34.198	0	2.2	3.2	94.6	100
369 (A1G)--V	34.968	4.8	3.3	0.4	91.5	100
370 (EU)--V	35.167	1.1	6.6	4.6	87.6	100
371 (EU)--V	35.167	1.1	6.6	4.6	87.6	100
372 (B2U)--V	35.284	0	7.9	8.5	83.6	100
373 (A2G)--V	35.448	0	0.7	14.8	84.5	100

374 (EG)--V	35.698	0.1	5.7	14.1	80	100
375 (EG)--V	35.698	0.1	5.7	14.1	80	100
376 (EU)--V	36.096	0.2	3.3	10.7	85.8	100
377 (EU)--V	36.096	0.2	3.3	10.7	85.8	100
378 (A2U)--V	36.37	0.2	1	10.8	88.1	100
379 (B1G)--V	36.457	0.5	19.6	7.2	72.7	100
380 (B2G)--V	36.532	0	1.7	1.8	96.5	100
381 (EU)--V	37.256	0.1	1.5	11.1	87.3	100
382 (EU)--V	37.256	0.1	1.5	11.1	87.3	100
383 (A1U)--V	37.277	0	19.9	17.9	62.2	100
384 (EG)--V	37.328	0	8.7	9.3	82	100
385 (EG)--V	37.328	0	8.7	9.3	82	100
386 (B2U)--V	37.433	0	6.7	9.3	84	100
387 (A2G)--V	37.589	0	1	9.1	90	100
388 (B1G)--V	38.257	0	0.5	4.2	95.2	100
389 (B1U)--V	38.347	0	5.4	7.2	87.5	100
390 (EG)--V	38.463	0.2	5.3	7.6	86.9	100
391 (EG)--V	38.463	0.2	5.3	7.6	86.9	100
392 (A1U)--V	38.719	0	3.5	5.9	90.6	100
393 (A2U)--V	39.116	4.3	27.5	16.7	51.5	100
394 (B1G)--V	39.158	0	5.8	0.2	94	100
395 (A1G)--V	39.223	3.6	6.2	0.1	90.2	100
396 (EU)--V	39.237	0.1	3.4	0.7	95.8	100
397 (EU)--V	39.237	0.1	3.4	0.7	95.8	100
398 (EG)--V	39.335	1.8	18.5	7.8	71.9	100
399 (EG)--V	39.335	1.8	18.5	7.8	71.9	100
400 (EU)--V	39.866	0.3	6.6	0.1	93	100
401 (EU)--V	39.866	0.3	6.6	0.1	93	100
402 (B2U)--V	40.994	0	27.7	0.8	71.6	100
403 (A1G)--V	41.138	0.1	0.5	0	99.3	100
404 (A2G)--V	41.139	0	2.9	18.2	78.9	100
405 (B2G)--V	41.257	0	0	0.5	99.5	100
406 (EU)--V	41.373	0	0.9	1.7	97.4	100
407 (EU)--V	41.373	0	0.9	1.7	97.4	100
408 (B1G)--V	41.455	0	0.1	1.2	98.6	100
409 (EG)--V	41.916	0.1	3.9	5.5	90.5	100
410 (EG)--V	41.916	0.1	3.9	5.5	90.5	100
411 (A2U)--V	41.929	0.5	1.8	2.1	95.6	100
412 (B2U)--V	42.004	0	0.2	0.6	99.2	100
413 (EG)--V	42.26	0.4	12.7	11.8	75	100
414 (EG)--V	42.26	0.4	12.7	11.8	75	100
415 (A2U)--V	42.493	2.4	10.5	0.9	86.2	100
416 (B1U)--V	42.879	0	18.7	23.5	57.8	100
417 (B2U)--V	42.907	0	2.3	0.8	96.9	100
418 (EU)--V	42.985	0	1.4	0.9	97.8	100
419 (EU)--V	42.985	0	1.4	0.9	97.8	100
420 (EG)--V	43.185	0.2	4.9	2.3	92.6	100
421 (EG)--V	43.185	0.2	4.9	2.3	92.6	100
422 (A1U)--V	43.22	0	0	0	100	100
423 (B1U)--V	43.283	0	3.8	5.2	91	100
424 (EG)--V	43.321	0.6	14.9	8.3	76.2	100

425 (EG)--V	43.321	0.6	14.9	8.3	76.2	100
426 A2G)--V	43.533	0	4.4	0	95.6	100
427 (A2U)--V	44.169	7.5	37.7	6.3	48.5	100
428 (A2G)--V	44.733	0	2.6	4.6	92.8	100
429 (B2G)--V	45.613	0	0.1	1.4	98.5	100
430 (EU)--V	45.671	0.4	8.5	0.3	90.8	100
431 (EU)--V	45.671	0.4	8.5	0.3	90.8	100
432 (A1G)--V	45.905	0.1	44.8	0.7	54.5	100
433 (EU)--V	46.037	0.4	8.9	2	88.6	100
434 (EU)--V	46.037	0.4	8.9	2	88.6	100
435 (B1G)--V	47.484	0	36.2	3	60.8	100
436 A1G)--V	47.507	0.7	37.7	3.2	58.4	100
437 (B2G)--V	48.484	0	0.2	21.3	78.5	100
438 (EU)--V	49.406	0.6	0.8	45.2	53.4	100
439 (EU)--V	49.406	0.6	0.8	45.2	53.4	100
440 (A1G)--V	49.718	1.1	1.1	56.7	41.1	100
441 B1G)--V	50.364	0	43	10.5	46.5	100
442 (EU)--V	50.615	0.2	32.3	3.9	63.6	100
443 (EU)--V	50.615	0.2	32.3	3.9	63.6	100
444 (B1U)--V	50.686	0	1.4	12.8	85.8	100
445 (A1G)--V	50.765	0.5	43.4	2.7	53.4	100
446 (EG)--V	51.015	0	2.4	10.3	87.3	100
447 (EG)--V	51.015	0	2.4	10.3	87.3	100
448 (A1U)--V	51.512	0	3.6	2.7	93.6	100
449 (B1G)--V	52.034	0	52.1	1.5	46.4	100
450 (B2G)--V	52.325	0	0.1	5.2	94.7	100
451 (EU)--V	52.583	0	10.1	8.2	81.6	100
452 (EU)--V	52.583	0	10.1	8.2	81.6	100
453 (A1G)--V	52.602	0.1	11.8	10.9	77.2	100
454 (EU)--V	52.664	0.2	4.2	16.3	79.4	100
455 (EU)--V	52.664	0.2	4.2	16.3	79.4	100
456 A2G)--V	52.919	0	0.5	0	99.5	100
457 (A2U)--V	52.977	0.4	10.4	25.4	63.7	100
458 (A1G)--V	53.317	0.5	21.2	35.7	42.6	100
459 (EU)--V	53.784	0	3.7	0.7	95.5	100
460 (EU)--V	53.784	0	3.7	0.7	95.5	100
461 B1G)--V	53.853	0	30.8	5.3	63.9	100
462 (EG)--V	54.133	0.4	15.8	17.6	66.2	100
463 (EG)--V	54.133	0.4	15.8	17.6	66.2	100
464 (A2G)--V	54.289	0	0.1	0	99.8	100
465 (B2G)--V	54.47	0	0	1.5	98.5	100
466 (EU)--V	54.592	0	0.9	1.6	97.5	100
467 (EU)--V	54.592	0	0.9	1.6	97.5	100
468 (A1G)--V	55.132	0	10.4	34.8	54.8	100
469 (B2U)--V	55.27	0	25.8	11.3	62.8	100
470 (B1G)--V	55.297	0	12.5	5	82.4	100
471 (EU)--V	55.4	1.9	6.6	13.5	78	100
472 (EU)--V	55.4	1.9	6.6	13.5	78	100
473 (B1G)--V	55.757	0	2.1	0.7	97.2	100
474 (EU)--V	55.964	3.5	13.3	8.1	75.2	100
475 (EU)--V	55.964	3.5	13.3	8.1	75.2	100

476 (EU)--V	56.359	13	28.1	0.6	58.3	100
477 (EU)--V	56.359	13	28.1	0.6	58.3	100
478 (A2G)--V	56.633	0	0	0.7	99.3	100
479 (A1G)--V	56.821	0.6	6.8	11	81.7	100
480 (B2G)--V	57.388	0	0.4	7.8	91.8	100
481 B2U)--V	57.532	0	27.9	14.9	57.2	100
482 (EU)--V	57.649	0	1.9	0.7	97.3	100
483 (EU)--V	57.649	0	1.9	0.7	97.3	100
484 (EU)--V	58.502	0.1	11.1	6	82.7	100
485 (EU)--V	58.502	0.1	11.1	6	82.7	100
486 A1G)--V	58.628	0.1	18.6	13.6	67.7	100
487 (EG)--V	58.832	0.9	28.3	18	52.8	100
488 (EG)--V	58.832	0.9	28.3	18	52.8	100
489 (B1G)--V	58.983	0	29.4	4.5	66.1	100
490 (A2G)--V	59.805	0	7.1	4.4	88.5	100
491 B1U)--V	59.992	0	2.3	29	68.7	100
492 (A2U)--V	60.081	0.3	4.6	20.8	74.2	100
493 (EG)--V	60.103	1.9	5.4	20	72.7	100
494 (EG)--V	60.103	1.9	5.4	20	72.7	100
495 (A1U)--V	60.124	0	24.7	10.9	64.4	100
496 B2G)--V	60.277	0	0.2	0.1	99.7	100
497 (EU)--V	60.596	0.1	0.7	1.3	98	100
498 (EU)--V	60.596	0.1	0.7	1.3	98	100
499 (EU)--V	60.7	0	2.2	4.2	93.5	100
500 (EU)--V	60.7	0	2.2	4.2	93.5	100
501 A2G)--V	60.805	0	1.9	2.1	96.1	100
502 (B1G)--V	61.343	0	4.1	8.6	87.3	100
503 (B2G)--V	61.442	0	0.4	7.4	92.1	100
504 (EU)--V	61.754	0.1	0.9	3.8	95.3	100
505 (EU)--V	61.754	0.1	0.9	3.8	95.3	100
506 A1G)--V	62.073	0.9	4.9	0.8	93.4	100
507 (EG)--V	62.425	8.4	13	2.9	75.7	100
508 (EG)--V	62.425	8.4	13	2.9	75.7	100
509 (B1U)--V	62.702	0	9.7	13.1	77.2	100
510 (A1U)--V	63.621	0	6	5.2	88.8	100
511 (EG)--V	63.631	67	9.2	1.9	21.9	100
512 (EG)--V	63.631	67	9.2	1.9	21.9	100
513 (A2G)--V	63.644	0	0	0.7	99.2	100
514 (B2U)--V	63.733	0	1	0	99	100
515 (EU)--V	63.924	0	4.7	8.1	87.1	100
516 (EU)--V	63.924	0	4.7	8.1	87.1	100
517 (EG)--V	64.334	1	9.2	0.1	89.7	100
518 (EG)--V	64.334	1	9.2	0.1	89.7	100
519 (B1U)--V	64.436	0	6.7	1.5	91.8	100
520 (EG)--V	64.671	7.3	2.3	6.6	83.8	100
521 (EG)--V	64.671	7.3	2.3	6.6	83.8	100
522 (A2U)--V	64.694	0.3	34.6	5.6	59.5	100
523 (A2U)--V	64.818	0.1	7.1	1.5	91.4	100
524 (A1U)--V	64.949	0	0.2	5	94.8	100
525 (B2G)--V	64.992	0	0.2	10.7	89.1	100
526 A2G)--V	65.18	0	4.1	1.6	94.3	100

527 (EU)--V	65.543	2.2	13.4	13.6	70.8	100
528 (EU)--V	65.543	2.2	13.4	13.6	70.8	100
529 (B1G)--V	65.684	0	35.9	16.5	47.6	100
530 (B2U)--V	65.852	0	2.3	1.2	96.5	100
531 (EG)--V	65.881	0.1	8.1	4.6	87.2	100
532 (EG)--V	65.881	0.1	8.1	4.6	87.2	100
533 (A1G)--V	66.364	0.1	1.3	17.7	80.9	100
534 (B1U)--V	67.765	0	18.3	1.7	80.1	100
535 (EU)--V	67.767	0.1	2.1	28	69.8	100
536 (EU)--V	67.767	0.1	2.1	28	69.8	100
537 (B2G)--V	67.959	5.6	2.9	17.9	73.6	100
538 (A2G)--V	68.519	0	0.1	0	99.9	100
539 (EG)--V	68.831	1	15.8	8.5	74.7	100
540 (EG)--V	68.831	1	15.8	8.5	74.7	100
541 (EU)--V	68.927	0	0.2	0.5	99.2	100
542 (EU)--V	68.927	0	0.2	0.5	99.2	100
543 (B2G)--V	68.994	0	1.9	24	74	100
544 (B1G)--V	69.268	0	2.1	0	97.9	100
545 (B2G)--V	70.193	0.9	6.5	10	82.5	100
546 A1U)--V	71.051	0	2.7	6.8	90.5	100
547 (A2U)--V	71.201	0.2	9	18.9	72	100
548 (A1G)--V	71.246	1.7	15.6	0.8	81.9	100
549 (EU)--V	71.346	0.2	8.6	12.1	79.1	100
550 (EU)--V	71.346	0.2	8.6	12.1	79.1	100
551 (EG)--V	72.315	0	7.8	10	82.2	100
552 (EG)--V	72.315	0	7.8	10	82.2	100
553 (A1U)--V	73.451	0	13.5	12.3	74.3	100
554 (B1U)--V	73.563	0	12.6	8.4	79	100
555 (A1G)--V	74.709	2.5	21.1	35	41.4	100
556 A2G)--V	74.831	0	0.5	0.2	99.3	100
557 (B1G)--V	74.848	0.6	58.6	4.1	36.7	100
558 (EU)--V	75.154	0	0.2	0.3	99.5	100
559 (EU)--V	75.154	0	0.2	0.3	99.5	100
560 (B2G)--V	75.284	0	0.3	0.1	99.6	100
561 (EG)--V	75.397	0.4	7	10.5	82.1	100
562 (EG)--V	75.397	0.4	7	10.5	82.1	100
563 (EU)--V	75.744	0.1	20.9	11.5	67.5	100
564 (EU)--V	75.744	0.1	20.9	11.5	67.5	100
565 (B1G)--V	75.957	0	1.2	0.6	98.2	100
566 (EU)--V	76.223	0.1	27	23.6	49.3	100
567 (EU)--V	76.223	0.1	27	23.6	49.3	100
568 (B1U)--V	76.241	0	0.2	4.1	95.7	100
569 (A1G)--V	76.255	1.1	15.5	25.8	57.6	100
570 (A2G)--V	76.328	0	4.2	2.8	93	100
571 (EU)--V	76.383	0	12.3	10.2	77.5	100
572 (EU)--V	76.383	0	12.3	10.2	77.5	100
573 (B1G)--V	76.511	0	27.9	8.1	63.9	100
574 (B2U)--V	77.421	0	15.8	31	53.2	100
575 (A1G)--V	77.466	5	20.5	8.6	66	100
576 A1U)--V	77.56	0	5.6	16.9	77.5	100
577 (EU)--V	77.594	0.1	44.1	11.5	44.3	100

578 (EU)--V	77.594	0.1	44.1	11.5	44.3	100
579 (EG)--V	77.626	0.3	10.1	22.5	67.1	100
580 (EG)--V	77.626	0.3	10.1	22.5	67.1	100
581 B1G)--V	77.651	0.1	31.5	4.6	63.7	100
582 (A1G)--V	77.944	2.1	55.6	12.7	29.6	100
583 (B2G)--V	78.692	0.1	0.5	8.2	91.3	100
584 (B2G)--V	79.083	0.2	5.2	19.6	75	100
585 (EU)--V	79.39	0	1.1	5.6	93.3	100
586 (EU)--V	79.39	0	1.1	5.6	93.3	100
587 (A2G)--V	79.872	0	0.5	5.9	93.7	100
588 (B1G)--V	80.221	2	48.1	3.8	46	100
589 (B2G)--V	80.47	0	0.1	0.9	99.1	100
590 (EU)--V	81.148	0	4	4.7	91.2	100
591 (EU)--V	81.148	0	4	4.7	91.2	100
592 (EU)--V	82.419	0.1	7.4	3.9	88.6	100
593 (EU)--V	82.419	0.1	7.4	3.9	88.6	100
594 (A2G)--V	82.702	0	1.3	2.1	96.7	100
595 (A1G)--V	82.884	0.3	21.7	25.1	53	100
596 (EU)--V	83.233	0.3	6.2	8.3	85.2	100
597 (EU)--V	83.233	0.3	6.2	8.3	85.2	100
598 (B2G)--V	84.448	0	0.2	8.4	91.5	100
599 (B1G)--V	85.24	1	7.2	6.7	85	100
600 (A2G)--V	85.355	0	0.2	0.1	99.7	100
601 (EU)--V	86.212	0.1	10.6	10.8	78.5	100
602 (EU)--V	86.212	0.1	10.6	10.8	78.5	100
603 (A1G)--V	86.482	0.7	4.4	6	88.9	100
604 (A2G)--V	87.15	0	19.7	5.7	74.6	100
605 (B2G)--V	88.465	0	2.4	2.7	94.9	100
606 (EU)--V	88.876	0	1.3	6.4	92.3	100
607 (EU)--V	88.876	0	1.3	6.4	92.3	100
608 (EU)--V	91.34	0.2	6.8	19.9	73.1	100
609 (EU)--V	91.34	0.2	6.8	19.9	73.1	100
610 (B1G)--V	92.889	1.1	5.5	26.2	67.2	100
611 A1G)--V	94.725	0.5	3.8	55.3	40.5	100
612 (B2G)--V	95.092	0	1	2	97	100
613 (EU)--V	96.322	0	1.5	3.1	95.3	100
614 (EU)--V	96.322	0	1.5	3.1	95.3	100
615 (A2G)--V	97.025	0	7.1	12.6	80.3	100
616 A2G)--V	97.191	0	2.2	2	95.7	100
617 (EU)--V	99.141	0	5.6	4.6	89.8	100
618 (EU)--V	99.141	0	5.6	4.6	89.8	100
619 (B2G)--V	99.833	0	4	3.2	92.7	100

### BHandHLYP Exchange Correlation Functional

Orbital	Index	E, eV	Zn	NZn	Nmeso	Pc	Total
	1 A1G)--O	-9512.07	100	0	0	0	100
	2 (A1G)--O	-1171.05	100	0	0	0	100
	3 (A2U)--O	-1030.36	100	0	0	0	100



4 (EU)--O	-1030.18	100	0	0	0	100
5 (EU)--O	-1030.18	100	0	0	0	100
6 B1G)--O	-403.437	0	99.9	0	0.1	100
7 (EU)--O	-403.437	0	99.9	0	0.1	100
8 (EU)--O	-403.437	0	99.9	0	0.1	100
9 (A1G)--O	-403.437	0	99.9	0	0.1	100
10 (B2G)--O	-403.263	0	0	99.8	0.2	100
11 (EU)--O	-403.263	0	0	99.9	0.1	100
12 (EU)--O	-403.263	0	0	99.9	0.1	100
13 (A1G)--O	-403.263	0	0	99.9	0.1	100
14 (B2G)--O	-290.53	0	0	0.1	99.9	100
15 (EU)--O	-290.53	0	0	0	99.9	100
16 (EU)--O	-290.53	0	0	0	99.9	100
17 (A2G)--O	-290.529	0	0	0	100	100
18 (EU)--O	-290.529	0	0	0	100	100
19 (EU)--O	-290.529	0	0	0	100	100
20 (A1G)--O	-290.529	0	0	0	100	100
21 B1G)--O	-290.529	0	0	0	100	100
22 (EU)--O	-288.547	0	0	0	100	100
23 (EU)--O	-288.547	0	0	0	100	100
24 (B1G)--O	-288.547	0	0	0	100	100
25 (A1G)--O	-288.547	0	0	0	100	100
26 A2G)--O	-288.543	0	0	0	100	100
27 (EU)--O	-288.543	0	0	0	100	100
28 (EU)--O	-288.543	0	0	0	100	100
29 (B2G)--O	-288.543	0	0	0	100	100
30 (EU)--O	-288.528	0	0	0	100	100
31 (EU)--O	-288.528	0	0	0	100	100
32 (A1G)--O	-288.528	0	0	0	100	100
33 (B1G)--O	-288.528	0	0	0	100	100
34 (B1G)--O	-288.512	0	0	0	100	100
35 (EU)--O	-288.512	0	0	0	100	100
36 (EU)--O	-288.512	0	0	0	100	100
37 (A1G)--O	-288.512	0	0	0	100	100
38 (A2G)--O	-288.512	0	0	0	100	100
39 (EU)--O	-288.512	0	0	0	100	100
40 (EU)--O	-288.512	0	0	0	100	100
41 B2G)--O	-288.512	0	0	0	100	100
42 (B2G)--O	-288.496	0	0	0	100	100
43 (EU)--O	-288.496	0	0	0	100	100
44 (EU)--O	-288.496	0	0	0	100	100
45 (A2G)--O	-288.496	0	0	0	100	100
46 A1G)--O	-139.378	100	0	0	0	100
47 (A2U)--O	-93.838	100	0	0	0	100
48 (EU)--O	-93.625	100	0	0	0	100
49 (EU)--O	-93.625	100	0	0	0	100
50 (A1G)--O	-30.99	0.4	39.4	26.1	34.2	100
51 (EU)--O	-30.561	0.2	38.2	26.3	35.4	100
52 (EU)--O	-30.561	0.2	38.2	26.3	35.4	100
53 (B1G)--O	-29.699	0.2	59.5	0.8	39.5	100
54 (B2G)--O	-29.128	0	1.6	70.5	27.9	100

55 (EU)--O	-27.867	0	18.5	49.9	31.6	100
56 (EU)--O	-27.867	0	18.5	49.9	31.6	100
57 (A1G)--O	-26.931	0.1	15.7	48.6	35.6	100
58 (A1G)--O	-26.487	0.4	25.2	11	63.5	100
59 (EU)--O	-26.477	0.1	15.5	1.3	83.1	100
60 (EU)--O	-26.477	0.1	15.5	1.3	83.1	100
61 B1G)--O	-26.463	0.1	13.8	0	86	100
62 (A2G)--O	-24.064	0	2.4	5.8	91.7	100
63 (A1G)--O	-23.725	0.6	12.3	0.4	86.8	100
64 (EU)--O	-23.695	0.1	13.9	3.4	82.5	100
65 (EU)--O	-23.695	0.1	13.9	3.4	82.5	100
66 (EU)--O	-23.573	0	4.3	1.4	94.3	100
67 (EU)--O	-23.573	0	4.3	1.4	94.3	100
68 (B1G)--O	-23.57	0.6	19	0.5	79.8	100
69 (B2G)--O	-23.49	0	0	1.8	98.2	100
70 (A2G)--O	-22.417	0	6.2	9.7	84.1	100
71 (EU)--O	-21.582	0	7.8	19.3	72.8	100
72 (EU)--O	-21.582	0	7.8	19.3	72.8	100
73 (B1G)--O	-19.981	2.7	14.6	15.2	67.5	100
74 (A1G)--O	-19.872	2.3	11.7	0.2	85.8	100
75 (EU)--O	-19.684	0.2	10.5	0.3	89.1	100
76 (EU)--O	-19.684	0.2	10.5	0.3	89.1	100
77 (B2G)--O	-19.559	0.1	3.2	12.5	84.2	100
78 (B1G)--O	-19.311	1	2.3	15.8	80.9	100
79 (EU)--O	-18.628	0	5.7	4.3	90	100
80 (EU)--O	-18.628	0	5.7	4.3	90	100
81 B2G)--O	-18.489	4.7	31.5	21.4	42.3	100
82 (A2G)--O	-18.353	0	6.4	2.3	91.4	100
83 (A1G)--O	-17.4	9.2	11.6	1.4	77.9	100
84 (EU)--O	-17.147	0	18.4	11.4	70.2	100
85 (EU)--O	-17.147	0	18.4	11.4	70.2	100
86 B1G)--O	-17.053	50.4	16.3	3	30.3	100
87 (EU)--O	-16.639	0.3	18	21.6	60.1	100
88 (EU)--O	-16.639	0.3	18	21.6	60.1	100
89 (B1G)--O	-16.023	39.9	3.9	2.6	53.6	100
90 (A1G)--O	-15.994	72	10.1	0.6	17.4	100
91 B2G)--O	-15.898	16.6	2.9	1.3	79.2	100
92 (EG)--O	-15.833	95.6	3.4	0.2	0.7	100
93 (EG)--O	-15.833	95.6	3.4	0.2	0.7	100
94 (A2G)--O	-15.623	0	30.6	16.4	53	100
95 (EU)--O	-15.205	0	2.9	5	92	100
96 (EU)--O	-15.205	0	2.9	5	92	100
97 (B2G)--O	-15.182	59.4	4.4	1.5	34.7	100
98 (A1G)--O	-14.781	30.4	7.8	1.6	60.3	100
99 (EU)--O	-14.691	0.6	13.5	0.8	85.2	100
100 (EU)--O	-14.691	0.6	13.5	0.8	85.2	100
101 A2G)--O	-14.646	0	0.4	9.1	90.5	100
102 (A2U)--O	-14.434	0.4	27.6	19	53	100
103 (B1G)--O	-14.394	7.9	7	0.8	84.3	100
104 (A1G)--O	-14.008	2.6	3.5	4	89.9	100
105 (EU)--O	-13.92	0	1.2	1.7	97	100

106 (EU)--O	-13.92	0	1.2	1.7	97	100
107 (B2G)--O	-13.909	0.1	0	1.3	98.6	100
108 (EG)--O	-13.832	8.4	20.6	16.7	54.3	100
109 (EG)--O	-13.832	8.4	20.6	16.7	54.3	100
110 (A2G)--O	-13.589	0	0.6	4.2	95.3	100
111 (EU)--O	-13.501	0.3	6.2	4.7	88.8	100
112 (EU)--O	-13.501	0.3	6.2	4.7	88.8	100
113 (B1G)--O	-13.224	4.7	2.2	4.6	88.5	100
114 (B2U)--O	-13.036	0	29.2	0	70.7	100
115 (A1G)--O	-12.735	23.6	26	6.8	43.6	100
116 B1U)--O	-11.984	0	0	53.3	46.7	100
117 (B2G)--O	-11.908	0.1	0.1	2.2	97.6	100
118 (EU)--O	-11.82	0.1	2.8	3.7	93.5	100
119 (EU)--O	-11.82	0.1	2.8	3.7	93.5	100
120 (A2G)--O	-11.579	0	2	1.2	96.8	100
121 (EU)--O	-11.477	3.2	36.4	3.7	56.7	100
122 (EU)--O	-11.477	3.2	36.4	3.7	56.7	100
123 (EG)--O	-11.417	0.4	3.6	12.6	83.3	100
124 (EG)--O	-11.417	0.4	3.6	12.6	83.3	100
125 (A2U)--O	-11.402	0.3	8.2	3.5	88	100
126 A1G)--O	-11.393	0	1.7	3.8	94.4	100
127 (B1G)--O	-11.029	1.2	2.1	2.8	93.9	100
128 (EU)--O	-10.992	1.5	14.9	7.7	76	100
129 (EU)--O	-10.992	1.5	14.9	7.7	76	100
130 (B2U)--O	-10.924	0	29.8	0	70.2	100
131 A1G)--O	-10.204	0.4	16.2	56.5	27	100
132 (EG)--O	-9.977	1	25	24	50	100
133 (EG)--O	-9.977	1	25	24	50	100
134 (EU)--O	-9.349	0.3	19	50.7	30	100
135 (EU)--O	-9.349	0.3	19	50.7	30	100
136 B2G)--O	-8.84	0.4	13.1	62.8	23.7	100
137 (A1U)--O	-8.614	0	0	0	100	100
138 (B1G)--O	-8.531	15.6	59	1	24.4	100
139 (A2U)--O	-8.201	2.2	46.2	20	31.6	100
140 (B1U)--O	-8.043	0	0	5.1	94.9	100
141 (EG)--O	-8.001	0	1.3	10.1	88.5	100
142 (EG)--O	-8.001	0	1.3	10.1	88.5	100
143 (EG)--O	-7.837	0.8	26	0.8	72.5	100
144 (EG)--O	-7.837	0.8	26	0.8	72.5	100
145 (B2U)--O	-7.783	0	24.2	0	75.8	100
146 A2U)--O	-7.741	0.2	6.9	39.7	53.2	100
147 (A1U)--O	-5.26	0	0.1	0.1	99.8	100
148 (EG)--V	-2.001	0.2	13	17.9	68.9	100
149 (EG)--V	-2.001	0.2	13	17.9	68.9	100
150 (B1U)--V	0.064	0	0	21.7	78.3	100
151 B2U)--V	0.351	0	18	0	81.9	100
152 (A2U)--V	0.477	13.8	0.2	5.6	80.4	100
153 (EG)--V	0.705	0.1	4.8	3.4	91.8	100
154 (EG)--V	0.705	0.1	4.8	3.4	91.8	100
155 (A2U)--V	1.739	65	9.1	0.2	25.6	100
156 A1G)--V	1.906	81.9	9.9	0.1	8.1	100

157 (A1U)--V	2.108	0	0	0	100	100
158 (EG)--V	2.206	0	1.8	1.1	97.1	100
159 (EG)--V	2.206	0	1.8	1.1	97.1	100
160 (B2U)--V	2.958	0	19.4	0.1	80.5	100
161 B1U)--V	3.281	0	0.1	19.9	80	100
162 (EU)--V	3.47	77.3	5.2	1.4	16.1	100
163 (EU)--V	3.47	77.3	5.2	1.4	16.1	100
164 (A1G)--V	3.907	0.4	0	1.2	98.4	100
165 (EU)--V	4.029	2.6	0.1	0.2	97.1	100
166 (EU)--V	4.029	2.6	0.1	0.2	97.1	100
167 (B1G)--V	4.121	0	0	0.1	99.9	100
168 (EG)--V	4.894	0.1	14	16	69.9	100
169 (EG)--V	4.894	0.1	14	16	69.9	100
170 (B2G)--V	4.929	0	0.7	0.1	99.2	100
171 A2U)--V	5.112	45.3	9.2	13.6	31.9	100
172 (EU)--V	5.169	0.1	0.8	0.3	98.9	100
173 (EU)--V	5.169	0.1	0.8	0.3	98.9	100
174 (A1G)--V	5.416	13.1	0.3	8.3	78.3	100
175 (A2G)--V	5.473	0	0.6	0.1	99.3	100
176 (EU)--V	5.852	0.4	0	2.3	97.2	100
177 (EU)--V	5.852	0.4	0	2.3	97.2	100
178 (B2G)--V	5.894	0	0	3.2	96.7	100
179 (A1G)--V	6.323	41.5	1.8	1.2	55.5	100
180 (EU)--V	6.357	0.2	0.9	0.1	98.9	100
181 (EU)--V	6.357	0.2	0.9	0.1	98.9	100
182 (B1G)--V	6.366	0	2.3	0	97.7	100
183 (A2G)--V	6.465	0	0	0	99.9	100
184 (A1U)--V	6.784	0	0	0	100	100
185 (B1U)--V	6.977	0	0	4.5	95.4	100
186 (EG)--V	6.985	0	0.9	4.2	94.9	100
187 (EG)--V	6.985	0	0.9	4.2	94.9	100
188 (B2G)--V	7.418	0.1	2.3	18.8	78.8	100
189 (EU)--V	7.429	4.4	10.8	6.6	78.3	100
190 (EU)--V	7.429	4.4	10.8	6.6	78.3	100
191 A1G)--V	7.86	0.1	0.7	2	97.2	100
192 (B1G)--V	8.01	0	32.7	2.7	64.6	100
193 (A2U)--V	8.201	72.7	7	3.8	16.5	100
194 (EU)--V	8.421	0.2	0.6	1.3	97.9	100
195 (EU)--V	8.421	0.2	0.6	1.3	97.9	100
196 A2G)--V	8.452	0	5.6	0.5	94	100
197 (B2G)--V	8.647	0	0.4	10.5	89	100
198 (EU)--V	8.706	0.5	0.4	5.5	93.6	100
199 (EU)--V	8.706	0.5	0.4	5.5	93.6	100
200 (A2G)--V	8.901	0	0	0	99.9	100
201 B1G)--V	9.07	0	0.7	0	99.3	100
202 (EU)--V	9.39	0.9	2.7	1.8	94.7	100
203 (EU)--V	9.39	0.9	2.7	1.8	94.7	100
204 (A1G)--V	9.507	4.9	6.7	22	66.4	100
205 (A1G)--V	9.854	5.1	0.6	4.5	89.8	100
206 (EU)--V	9.961	0.7	10.9	3.5	85	100
207 (EU)--V	9.961	0.7	10.9	3.5	85	100

208 (B1G)--V	10.547	0	0.5	0.2	99.3	100
209 (B2G)--V	10.721	0	1.2	4.6	94.2	100
210 (EU)--V	10.85	0.3	3.1	16.5	80	100
211 (EU)--V	10.85	0.3	3.1	16.5	80	100
212 (A1G)--V	11.056	0.3	3.5	2.9	93.3	100
213 (EU)--V	11.162	1.4	4.7	0.4	93.5	100
214 (EU)--V	11.162	1.4	4.7	0.4	93.5	100
215 (B2G)--V	11.341	0	3.2	24.7	72.1	100
216 B1G)--V	11.695	0	5.2	0	94.7	100
217 (B2G)--V	12.151	0	3	9	87.9	100
218 (A1G)--V	12.362	1.2	19.1	11.8	67.8	100
219 (EU)--V	12.397	2.2	3.8	16	78	100
220 (EU)--V	12.397	2.2	3.8	16	78	100
221 A2G)--V	12.924	0	6.1	8.4	85.5	100
222 (B1G)--V	13.356	0	19.6	9.4	71	100
223 (EU)--V	13.512	2.1	9.7	10.8	77.3	100
224 (EU)--V	13.512	2.1	9.7	10.8	77.3	100
225 (A2G)--V	13.621	0	0.1	1.3	98.6	100
226 (EU)--V	13.829	0.8	1.4	3	94.9	100
227 (EU)--V	13.829	0.8	1.4	3	94.9	100
228 (EU)--V	15.621	1.9	3.2	3.3	91.7	100
229 (EU)--V	15.621	1.9	3.2	3.3	91.7	100
230 (EG)--V	15.812	0	1.3	1.3	97.4	100
231 (EG)--V	15.812	0	1.3	1.3	97.4	100
232 (A2G)--V	15.964	0	0.1	5.1	94.8	100
233 (B2U)--V	16.045	0	0.4	0	99.5	100
234 (B2G)--V	16.062	0	0.3	0	99.7	100
235 (A2U)--V	16.152	3.6	0.2	0.6	95.5	100
236 B1G)--V	16.619	0	34.1	5	60.8	100
237 (A1G)--V	16.661	0.6	4.8	1.5	93.1	100
238 (EG)--V	16.72	0	1.7	1.5	96.8	100
239 (EG)--V	16.72	0	1.7	1.5	96.8	100
240 (EU)--V	16.778	0.2	0.8	2.4	96.6	100
241 (EU)--V	16.778	0.2	0.8	2.4	96.6	100
242 (B1U)--V	16.986	0	0	3.9	96.1	100
243 (A2G)--V	17.004	0	1	3.8	95.2	100
244 (EU)--V	17.192	0.4	0.7	1	98	100
245 (EU)--V	17.192	0.4	0.7	1	98	100
246 B1G)--V	17.33	0	4.7	1	94.3	100
247 (B2G)--V	17.376	0	0.4	1.3	98.3	100
248 (EU)--V	17.54	0	0.4	0.9	98.6	100
249 (EU)--V	17.54	0	0.4	0.9	98.6	100
250 (B2U)--V	17.547	0	1.3	0.1	98.7	100
251 A2U)--V	17.616	8.6	1.5	1.3	88.6	100
252 (A1G)--V	17.717	1.5	0.7	10.1	87.6	100
253 (EG)--V	17.839	0	0.5	1.4	98.2	100
254 (EG)--V	17.839	0	0.5	1.4	98.2	100
255 (A2G)--V	17.847	0	0.2	0.7	99	100
256 B2G)--V	17.875	0	1.1	1.5	97.4	100
257 (EU)--V	17.932	0.1	0.9	0.7	98.3	100
258 (EU)--V	17.932	0.1	0.9	0.7	98.3	100

259 (A1U)--V	17.971	0	0	0	100	100
260 (B1G)--V	18.031	0	24.5	1.2	74.3	100
261 A1G)--V	18.58	1.3	16.7	1.6	80.4	100
262 (EU)--V	18.621	0.4	19.5	12.2	67.9	100
263 (EU)--V	18.621	0.4	19.5	12.2	67.9	100
264 (A1G)--V	18.707	0.4	21.6	13.9	64.1	100
265 (A2G)--V	18.809	0	0.7	1	98.3	100
266 B1U)--V	18.814	0	0	1.1	98.9	100
267 (B1G)--V	18.817	0	2.5	1.6	95.9	100
268 (EU)--V	18.827	0.1	0.7	1.4	97.7	100
269 (EU)--V	18.827	0.1	0.7	1.4	97.7	100
270 (B2G)--V	18.864	0	1.1	4.7	94.2	100
271 (EG)--V	19.077	0	2.9	0.6	96.4	100
272 (EG)--V	19.077	0	2.9	0.6	96.4	100
273 (EU)--V	19.098	1.2	24.1	8.1	66.5	100
274 (EU)--V	19.098	1.2	24.1	8.1	66.5	100
275 (A1G)--V	19.371	1.2	4.9	24	69.9	100
276 A2G)--V	19.815	0	1.1	3.5	95.3	100
277 (A2U)--V	19.84	2.6	1	1.2	95.1	100
278 (EG)--V	19.869	0	0.9	3	96	100
279 (EG)--V	19.869	0	0.9	3	96	100
280 (B2U)--V	20.007	0	1.4	0	98.6	100
281 A1U)--V	20.033	0	0	0	100	100
282 (EU)--V	20.086	1.9	3.6	1.7	92.7	100
283 (EU)--V	20.086	1.9	3.6	1.7	92.7	100
284 (EU)--V	20.384	1	1.5	14.7	82.9	100
285 (EU)--V	20.384	1	1.5	14.7	82.9	100
286 B2G)--V	20.429	0	0.5	14	85.5	100
287 (B1U)--V	20.777	0	0	2.2	97.8	100
288 (EG)--V	20.9	0	0.4	0.3	99.3	100
289 (EG)--V	20.9	0	0.4	0.3	99.3	100
290 (B1G)--V	21.078	0.1	9.6	10.6	79.8	100
291 A2U)--V	21.09	0.5	0.4	2.8	96.4	100
292 (A1G)--V	21.587	5.4	21.3	4.4	68.9	100
293 (B2U)--V	22.306	0	0.9	0	99.1	100
294 (EG)--V	22.386	0	0.7	1.1	98.2	100
295 (EG)--V	22.386	0	0.7	1.1	98.2	100
296 A1U)--V	22.549	0	0	0	100	100
297 (EU)--V	22.84	5	14.1	6.8	74.1	100
298 (EU)--V	22.84	5	14.1	6.8	74.1	100
299 (B1U)--V	23.182	0	0	3.1	96.9	100
300 (EG)--V	23.879	0.2	27.4	5.9	66.5	100
301 (EG)--V	23.879	0.2	27.4	5.9	66.5	100
302 (B2G)--V	24.155	0	0.6	3.2	96.2	100
303 (EU)--V	24.318	0.1	1.5	1.8	96.6	100
304 (EU)--V	24.318	0.1	1.5	1.8	96.6	100
305 (A1G)--V	24.406	0.1	0.5	1.2	98.3	100
306 A2U)--V	24.796	1.1	11.5	59.7	27.7	100
307 (B2G)--V	24.816	0	1.7	1.4	96.9	100
308 (EG)--V	24.875	0	4.9	1	94.1	100
309 (EG)--V	24.875	0	4.9	1	94.1	100

310 (A2G)--V	25.004	0	0.3	1.5	98.1	100
311 (EU)--V	25.061	0.1	0	1	98.9	100
312 (EU)--V	25.061	0.1	0	1	98.9	100
313 (A2G)--V	25.252	0	2	0.6	97.5	100
314 (EU)--V	25.484	0	1.1	0.2	98.7	100
315 (EU)--V	25.484	0	1.1	0.2	98.7	100
316 B1G)--V	25.53	0	1.4	0.7	97.9	100
317 (A1G)--V	25.723	0.5	10.3	7.7	81.4	100
318 (B2G)--V	25.734	0	0.8	13.2	86	100
319 (EU)--V	25.917	0.2	2.6	4.2	93	100
320 (EU)--V	25.917	0.2	2.6	4.2	93	100
321 B2G)--V	26.059	0	9.5	4.7	85.8	100
322 (A1U)--V	26.366	0	0	0	100	100
323 (B1G)--V	26.512	0	0.2	0.2	99.6	100
324 (EU)--V	26.519	0.1	1	3.6	95.3	100
325 (EU)--V	26.519	0.1	1	3.6	95.3	100
326 A2G)--V	26.536	0	0.3	7.3	92.3	100
327 (A1G)--V	26.682	2	2	23.3	72.7	100
328 (B2U)--V	26.72	0	70.7	0	29.2	100
329 (B1G)--V	27.265	0	19.8	11.9	68.3	100
330 (EG)--V	27.314	0.1	15	42.3	42.6	100
331 (EG)--V	27.314	0.1	15	42.3	42.6	100
332 (B1U)--V	27.36	0	0	65.4	34.6	100
333 (A1G)--V	27.375	0.8	10.3	6.5	82.4	100
334 (EU)--V	27.637	0.1	4.1	5.9	89.9	100
335 (EU)--V	27.637	0.1	4.1	5.9	89.9	100
336 (EU)--V	27.832	0.6	10.2	5.6	83.7	100
337 (EU)--V	27.832	0.6	10.2	5.6	83.7	100
338 (A2G)--V	28.022	0	0	0	100	100
339 (B1G)--V	28.138	0	0.3	0.2	99.6	100
340 (EU)--V	28.555	0.4	0.3	4.9	94.4	100
341 (EU)--V	28.555	0.4	0.3	4.9	94.4	100
342 (B2G)--V	29.115	0	0.4	1.3	98.2	100
343 (EU)--V	29.405	0.1	2.1	3.2	94.6	100
344 (EU)--V	29.405	0.1	2.1	3.2	94.6	100
345 (A2U)--V	29.497	4.6	44.3	15.8	35.2	100
346 A2G)--V	29.523	0	0	1.7	98.2	100
347 (B2G)--V	29.663	0	0.6	1.5	97.9	100
348 (B1G)--V	29.684	0	7.5	2.8	89.7	100
349 (EU)--V	29.968	0.2	5.2	3	91.6	100
350 (EU)--V	29.968	0.2	5.2	3	91.6	100
351 (EU)--V	30.322	0	4.4	5.5	90.1	100
352 (EU)--V	30.322	0	4.4	5.5	90.1	100
353 (A1G)--V	30.385	0	3.5	3.4	93.1	100
354 (A1G)--V	30.684	0.2	5.2	6.8	87.8	100
355 (B2G)--V	31.078	0	7.3	4.1	88.6	100
356 A2G)--V	31.578	0	0.7	0.3	98.9	100
357 (EU)--V	31.605	0	2.9	3.3	93.7	100
358 (EU)--V	31.605	0	2.9	3.3	93.7	100
359 (A2G)--V	32.724	0	3.5	3.1	93.4	100
360 (EU)--V	32.99	0.1	0.7	1.1	98.2	100

361 (EU)--V	32.99	0.1	0.7	1.1	98.2	100
362 (B1G)--V	33.009	0	0.9	15.5	83.6	100
363 (B2G)--V	33.21	0	0.8	3.8	95.3	100
364 (B1G)--V	33.368	0	4.6	11.6	83.8	100
365 (A1G)--V	33.756	0.7	5.9	3.8	89.7	100
366 (EU)--V	33.824	0.1	5.7	4.1	90.1	100
367 (EU)--V	33.824	0.1	5.7	4.1	90.1	100
368 (B2G)--V	34.179	0	2	4.7	93.3	100
369 (A1G)--V	35.05	4.7	3.2	0.4	91.6	100
370 (EU)--V	35.216	1	5.2	4.8	89	100
371 (EU)--V	35.216	1	5.2	4.8	89	100
372 (B2U)--V	35.258	0	7.7	8.2	84.2	100
373 (A2G)--V	35.48	0	0.7	14.7	84.6	100
374 (EG)--V	35.667	0.1	5.4	13.9	80.6	100
375 (EG)--V	35.667	0.1	5.4	13.9	80.6	100
376 (EU)--V	36.144	0.3	3.6	10.2	85.9	100
377 (EU)--V	36.144	0.3	3.6	10.2	85.9	100
378 (A2U)--V	36.304	0.2	0.9	10.7	88.1	100
379 (B2G)--V	36.55	0	1.7	1.8	96.5	100
380 (B1G)--V	36.603	0.4	18.7	7.2	73.7	100
381 A1U)--V	37.301	0	20.1	17.8	62.2	100
382 (EG)--V	37.303	0	8.9	9.5	81.5	100
383 (EG)--V	37.303	0	8.9	9.5	81.5	100
384 (EU)--V	37.33	0.1	1.5	11.3	87	100
385 (EU)--V	37.33	0.1	1.5	11.3	87	100
386 B2U)--V	37.393	0	6.9	9.6	83.6	100
387 (A2G)--V	37.579	0	1	9.1	89.9	100
388 (B1U)--V	38.319	0	5.3	7.2	87.5	100
389 (B1G)--V	38.355	0	0.5	4.1	95.3	100
390 (EG)--V	38.433	0.2	5.3	7.7	86.9	100
391 (EG)--V	38.433	0.2	5.3	7.7	86.9	100
392 (A1U)--V	38.686	0	3.4	6	90.6	100
393 (A2U)--V	39.093	4.3	27.7	16.7	51.4	100
394 (B1G)--V	39.238	0	5.9	0.2	93.9	100
395 (EU)--V	39.296	0.1	3.1	0.7	96.1	100
396 (EU)--V	39.296	0.1	3.1	0.7	96.1	100
397 (A1G)--V	39.307	3.6	6.2	0.1	90.1	100
398 (EG)--V	39.318	1.8	18.6	7.8	71.8	100
399 (EG)--V	39.318	1.8	18.6	7.8	71.8	100
400 (EU)--V	39.98	0.3	6.7	0.1	92.9	100
401 (EU)--V	39.98	0.3	6.7	0.1	92.9	100
402 (B2U)--V	40.968	0	27.7	0.8	71.5	100
403 (A1G)--V	41.008	0.1	0.6	0	99.3	100
404 (B2G)--V	41.218	0	0	0.5	99.5	100
405 (A2G)--V	41.229	0	2.9	17.7	79.4	100
406 (EU)--V	41.268	0.1	1	1.8	97.1	100
407 (EU)--V	41.268	0.1	1	1.8	97.1	100
408 (B1G)--V	41.336	0	0.1	1.3	98.6	100
409 (EG)--V	41.868	0.1	3.6	5.3	91	100
410 (EG)--V	41.868	0.1	3.6	5.3	91	100
411 A2U)--V	41.878	0.5	1.9	2.1	95.5	100



412 (B2U)--V	41.955	0	0.1	0.7	99.2	100
413 (EG)--V	42.23	0.4	12.3	11.5	75.8	100
414 (EG)--V	42.23	0.4	12.3	11.5	75.8	100
415 (A2U)--V	42.444	2.3	10.1	0.9	86.7	100
416 B2U)--V	42.849	0	2.4	0.8	96.9	100
417 (B1U)--V	42.862	0	18	22.5	59.5	100
418 (EU)--V	43.001	0	1.4	0.9	97.6	100
419 (EU)--V	43.001	0	1.4	0.9	97.6	100
420 (EG)--V	43.13	0.2	4.2	1.9	93.7	100
421 (EG)--V	43.13	0.2	4.2	1.9	93.7	100
422 (A1U)--V	43.161	0	0	0	100	100
423 (B1U)--V	43.233	0	4.7	6.4	88.8	100
424 (EG)--V	43.278	0.6	16.4	9.2	73.8	100
425 (EG)--V	43.278	0.6	16.4	9.2	73.8	100
426 A2G)--V	43.622	0	4.3	0.1	95.6	100
427 (A2U)--V	44.142	7.6	38	6.4	48.1	100
428 (A2G)--V	44.792	0	2.9	4.7	92.4	100
429 (B2G)--V	45.696	0	0.1	1.5	98.5	100
430 (EU)--V	45.725	0.4	8.4	0.4	90.9	100
431 (EU)--V	45.725	0.4	8.4	0.4	90.9	100
432 (A1G)--V	45.947	0.1	44.4	0.7	54.8	100
433 (EU)--V	46.138	0.4	8.9	2	88.6	100
434 (EU)--V	46.138	0.4	8.9	2	88.6	100
435 (A1G)--V	47.524	0.8	36.9	3.6	58.7	100
436 B1G)--V	47.548	0	36.3	3	60.7	100
437 (B2G)--V	48.55	0	0.2	21.1	78.8	100
438 (EU)--V	49.451	0.6	0.8	45.2	53.4	100
439 (EU)--V	49.451	0.6	0.8	45.2	53.4	100
440 (A1G)--V	49.751	1.1	1.2	56.3	41.4	100
441 B1G)--V	50.343	0	43.1	10.5	46.3	100
442 (EU)--V	50.591	0.2	31.6	3.8	64.5	100
443 (EU)--V	50.591	0.2	31.6	3.8	64.5	100
444 (B1U)--V	50.657	0	1.4	12.7	85.8	100
445 (A1G)--V	50.763	0.5	43.6	3.1	52.8	100
446 (EG)--V	50.985	0	2.4	10.3	87.3	100
447 (EG)--V	50.985	0	2.4	10.3	87.3	100
448 (A1U)--V	51.478	0	3.6	2.7	93.7	100
449 (B1G)--V	52.017	0	52.4	1.5	46.1	100
450 (B2G)--V	52.258	0	0.1	5.1	94.8	100
451 (EU)--V	52.55	0	10.6	7.9	81.5	100
452 (EU)--V	52.55	0	10.6	7.9	81.5	100
453 (A1G)--V	52.633	0.1	13.1	8.9	77.8	100
454 (EU)--V	52.648	0.1	3.9	15.5	80.5	100
455 (EU)--V	52.648	0.1	3.9	15.5	80.5	100
456 A2G)--V	52.838	0	0.5	0	99.5	100
457 (A2U)--V	52.956	0.4	10.5	25.4	63.6	100
458 (A1G)--V	53.306	0.5	21.1	35.8	42.6	100
459 (EU)--V	53.738	0	3.4	0.8	95.8	100
460 (EU)--V	53.738	0	3.4	0.8	95.8	100
461 B1G)--V	53.838	0	30.8	5.3	63.9	100
462 (EG)--V	54.108	0.4	15.8	17.6	66.2	100

463 (EG)--V	54.108	0.4	15.8	17.6	66.2	100
464 (A2G)--V	54.23	0	0.1	0	99.8	100
465 (B2G)--V	54.321	0	0	1.4	98.6	100
466 (EU)--V	54.471	0	1	1.5	97.5	100
467 (EU)--V	54.471	0	1	1.5	97.5	100
468 (A1G)--V	54.997	0	10.3	35.8	53.8	100
469 (B2U)--V	55.239	0	25.7	11.2	63	100
470 (B1G)--V	55.323	0	13.1	5.3	81.6	100
471 (EU)--V	55.341	1.7	6	16	76.3	100
472 (EU)--V	55.341	1.7	6	16	76.3	100
473 (B1G)--V	55.617	0	1.8	0.5	97.7	100
474 (EU)--V	55.893	2.3	13.6	9.3	74.8	100
475 (EU)--V	55.893	2.3	13.6	9.3	74.8	100
476 (EU)--V	56.4	15.3	30.7	0.7	53.3	100
477 (EU)--V	56.4	15.3	30.7	0.7	53.3	100
478 (A2G)--V	56.584	0	0	0.7	99.3	100
479 (A1G)--V	56.806	0.6	6.8	11.2	81.5	100
480 (B2G)--V	57.324	0	0.4	7.9	91.7	100
481 B2U)--V	57.533	0	28	15	57	100
482 (EU)--V	57.625	0	2.2	0.8	97	100
483 (EU)--V	57.625	0	2.2	0.8	97	100
484 (EU)--V	58.478	0.2	10.4	5.4	84	100
485 (EU)--V	58.478	0.2	10.4	5.4	84	100
486 A1G)--V	58.545	0.1	18.7	13.9	67.3	100
487 (EG)--V	58.824	0.9	28.2	18.1	52.9	100
488 (EG)--V	58.824	0.9	28.2	18.1	52.9	100
489 (B1G)--V	58.948	0	28.9	4.2	66.9	100
490 (A2G)--V	59.794	0	7.5	4.5	88.1	100
491 B1U)--V	59.963	0	2.3	28.9	68.8	100
492 (A2U)--V	60.048	0.3	4.7	20.8	74.2	100
493 (EG)--V	60.074	1.8	5.5	19.9	72.8	100
494 (EG)--V	60.074	1.8	5.5	19.9	72.8	100
495 (A1U)--V	60.101	0	24.6	10.9	64.5	100
496 B2G)--V	60.237	0	0.2	0.1	99.7	100
497 (EU)--V	60.534	0.1	0.8	1.6	97.5	100
498 (EU)--V	60.534	0.1	0.8	1.6	97.5	100
499 (EU)--V	60.681	0	2.1	4	93.9	100
500 (EU)--V	60.681	0	2.1	4	93.9	100
501 A2G)--V	60.78	0	2.1	2.2	95.8	100
502 (B1G)--V	61.328	0	4.2	8.7	87.1	100
503 (B2G)--V	61.409	0	0.4	7.3	92.3	100
504 (EU)--V	61.73	0.1	0.9	3.6	95.4	100
505 (EU)--V	61.73	0.1	0.9	3.6	95.4	100
506 A1G)--V	62.05	0.9	4.9	0.8	93.4	100
507 (EG)--V	62.42	7.7	12.7	3	76.6	100
508 (EG)--V	62.42	7.7	12.7	3	76.6	100
509 (B1U)--V	62.696	0	9.3	13.2	77.4	100
510 (A1U)--V	63.582	0	6	5.1	88.9	100
511 A2G)--V	63.638	0	0	0.7	99.2	100
512 (EG)--V	63.657	66.8	9.1	1.8	22.3	100
513 (EG)--V	63.657	66.8	9.1	1.8	22.3	100

514 (B2U)--V	63.701	0	1	0	99	100
515 (EU)--V	63.922	0	4.6	8	87.3	100
516 (EU)--V	63.922	0	4.6	8	87.3	100
517 (EG)--V	64.299	1	9.3	0.1	89.6	100
518 (EG)--V	64.299	1	9.3	0.1	89.6	100
519 (B1U)--V	64.392	0	6.9	1.4	91.8	100
520 (EG)--V	64.638	8.3	2.5	6.6	82.6	100
521 (EG)--V	64.638	8.3	2.5	6.6	82.6	100
522 (A2U)--V	64.69	0.2	29.8	6.4	63.6	100
523 (A2U)--V	64.791	0.1	13.4	0.7	85.8	100
524 (A1U)--V	64.92	0	0.2	5	94.8	100
525 (B2G)--V	64.98	0	0.2	10.8	89	100
526 A2G)--V	65.196	0	3.9	1.5	94.6	100
527 (EU)--V	65.554	2.2	13.5	13.5	70.7	100
528 (EU)--V	65.554	2.2	13.5	13.5	70.7	100
529 (B1G)--V	65.72	0	36.1	16.5	47.4	100
530 (B2U)--V	65.833	0	2.3	1.2	96.5	100
531 (EG)--V	65.86	0.1	8.2	4.5	87.2	100
532 (EG)--V	65.86	0.1	8.2	4.5	87.2	100
533 (A1G)--V	66.415	0.1	1.3	17.6	81	100
534 (B1U)--V	67.75	0	18.3	1.7	79.9	100
535 (EU)--V	67.824	0.2	2.1	27.5	70.3	100
536 (EU)--V	67.824	0.2	2.1	27.5	70.3	100
537 (B2G)--V	67.98	5.3	2.6	20.2	71.9	100
538 (A2G)--V	68.513	0	0.1	0	99.9	100
539 (EG)--V	68.825	1	15.8	8.6	74.6	100
540 (EG)--V	68.825	1	15.8	8.6	74.6	100
541 (EU)--V	68.93	0	0.2	0.7	99	100
542 (EU)--V	68.93	0	0.2	0.7	99	100
543 (B2G)--V	69.094	0	1.9	23.7	74.3	100
544 (B1G)--V	69.244	0	2	0	98	100
545 (B2G)--V	70.205	1	6.8	11.1	81	100
546 A1U)--V	71.032	0	2.8	6.8	90.4	100
547 (A2U)--V	71.191	0.2	9	18.9	72	100
548 (A1G)--V	71.216	1.6	15.5	0.7	82.2	100
549 (EU)--V	71.305	0.2	8.7	12.3	78.8	100
550 (EU)--V	71.305	0.2	8.7	12.3	78.8	100
551 (EG)--V	72.296	0	7.8	10	82.2	100
552 (EG)--V	72.296	0	7.8	10	82.2	100
553 (A1U)--V	73.443	0	13.4	12.1	74.5	100
554 (B1U)--V	73.542	0	12.6	8.3	79	100
555 (A1G)--V	74.715	2.4	20.7	34.6	42.2	100
556 A2G)--V	74.798	0	0.5	0.2	99.3	100
557 (B1G)--V	74.883	0.6	57.7	4.3	37.4	100
558 (EU)--V	75.104	0	0.1	0.3	99.6	100
559 (EU)--V	75.104	0	0.1	0.3	99.6	100
560 (B2G)--V	75.236	0	0.3	0	99.6	100
561 (EG)--V	75.378	0.4	6.9	10.4	82.4	100
562 (EG)--V	75.378	0.4	6.9	10.4	82.4	100
563 (EU)--V	75.71	0.1	19.8	11	69.1	100
564 (EU)--V	75.71	0.1	19.8	11	69.1	100

565 (B1G)--V	75.92	0	1.2	0.7	98.1	100
566 (EU)--V	76.188	0.1	27.1	25	47.8	100
567 (EU)--V	76.188	0.1	27.1	25	47.8	100
568 (B1U)--V	76.213	0	0.2	4.1	95.7	100
569 (A1G)--V	76.228	1.1	14.9	25.6	58.3	100
570 (A2G)--V	76.254	0	4.4	2.9	92.7	100
571 (EU)--V	76.364	0	12.9	10.6	76.5	100
572 (EU)--V	76.364	0	12.9	10.6	76.5	100
573 (B1G)--V	76.501	0	28.6	7.5	63.9	100
574 (B2U)--V	77.425	0	15.8	31	53.2	100
575 (A1G)--V	77.453	4.8	22.4	10.3	62.5	100
576 A1U)--V	77.549	0	5.7	17.1	77.2	100
577 (EU)--V	77.595	0.1	43.9	12.5	43.5	100
578 (EU)--V	77.595	0.1	43.9	12.5	43.5	100
579 (EG)--V	77.62	0.3	10.2	22.6	66.9	100
580 (EG)--V	77.62	0.3	10.2	22.6	66.9	100
581 B1G)--V	77.629	0.1	32.4	4.7	62.8	100
582 (A1G)--V	77.984	2.1	54.5	13.3	30.1	100
583 (B2G)--V	78.656	0	0.3	7.4	92.3	100
584 (B2G)--V	79.125	0.2	4.9	19.8	75.2	100
585 (EU)--V	79.351	0	1.2	5.7	93.1	100
586 (EU)--V	79.351	0	1.2	5.7	93.1	100
587 (A2G)--V	79.827	0	0.5	5.9	93.6	100
588 (B1G)--V	80.231	2	47.8	3.6	46.7	100
589 (B2G)--V	80.409	0	0.1	0.7	99.2	100
590 (EU)--V	81.102	0	3.9	4.6	91.5	100
591 (EU)--V	81.102	0	3.9	4.6	91.5	100
592 (EU)--V	82.395	0.1	7.4	3.9	88.6	100
593 (EU)--V	82.395	0.1	7.4	3.9	88.6	100
594 (A2G)--V	82.658	0	1.3	2.1	96.7	100
595 (A1G)--V	82.874	0.3	21.7	25.1	52.9	100
596 (EU)--V	83.219	0.3	6.1	8.1	85.5	100
597 (EU)--V	83.219	0.3	6.1	8.1	85.5	100
598 (B2G)--V	84.426	0	0.2	8.5	91.3	100
599 (B1G)--V	85.239	1	7.4	6.8	84.8	100
600 (A2G)--V	85.325	0	0.2	0.1	99.7	100
601 (EU)--V	86.199	0.1	10.8	11	78.2	100
602 (EU)--V	86.199	0.1	10.8	11	78.2	100
603 (A1G)--V	86.452	0.7	4.4	6.2	88.7	100
604 (A2G)--V	87.123	0	19.7	5.7	74.6	100
605 (B2G)--V	88.433	0	2.4	2.6	95	100
606 (EU)--V	88.855	0	1.3	6.4	92.3	100
607 (EU)--V	88.855	0	1.3	6.4	92.3	100
608 (EU)--V	91.31	0.2	6.9	20	72.9	100
609 (EU)--V	91.31	0.2	6.9	20	72.9	100
610 (B1G)--V	92.887	1.1	5.5	26.3	67.1	100
611 A1G)--V	94.718	0.5	3.8	55.4	40.4	100
612 (B2G)--V	95.034	0	1	2	97	100
613 (EU)--V	96.269	0	1.5	3.1	95.4	100
614 (EU)--V	96.269	0	1.5	3.1	95.4	100
615 (A2G)--V	96.999	0	5.5	10.6	83.8	100

616 A2G)--V	97.121	0	3.4	3.7	92.9	100
617 (EU)--V	99.107	0	5.8	4.7	89.5	100
618 (EU)--V	99.107	0	5.8	4.7	89.5	100
619 (B2G)--V	99.797	0	4.2	3.3	92.5	100

## Hartree-Fock

Orbital	Index	E, eV	Zn	NZn	Nmeso	Pc	Total	
	1 A1G)--O	-9613.44		100	0	0	0	100
	2 (A1G)--O	-1207.19		100	0	0	0	100
	3 (A2U)--O	-1059.46		100	0	0	0	100
	4 (EU)--O	-1059.3		100	0	0	0	100
	5 (EU)--O	-1059.3		100	0	0	0	100
	6 B1G)--O	-423.93		0	99.9	0	0.1	100
	7 (EU)--O	-423.93		0	99.9	0	0	100
	8 (EU)--O	-423.93		0	99.9	0	0	100
	9 (A1G)--O	-423.93		0	100	0	0	100
	10 (B2G)--O	-423.855		0	0	99.9	0.1	100
	11 (EU)--O	-423.855		0	0	99.9	0.1	100
	12 (EU)--O	-423.855		0	0	99.9	0.1	100
	13 (A1G)--O	-423.855		0	0	99.9	0	100
	14 (A2G)--O	-308.179		0	0	0	100	100
	15 (EU)--O	-308.179		0	0	0	100	100
	16 (EU)--O	-308.179		0	0	0	100	100
	17 (B2G)--O	-308.179		0	0	0	100	100
	18 (EU)--O	-308.178		0	0	0	100	100
	19 (EU)--O	-308.178		0	0	0	100	100
	20 (B1G)--O	-308.178		0	0	0	100	100
	21 A1G)--O	-308.178		0	0	0	100	100
	22 (EU)--O	-306.037		0	0	0	100	100
	23 (EU)--O	-306.037		0	0	0	100	100
	24 (B1G)--O	-306.037		0	0	0	100	100
	25 (A1G)--O	-306.037		0	0	0	100	100
	26 A2G)--O	-306.034		0	0	0	100	100
	27 (EU)--O	-306.034		0	0	0	100	100
	28 (EU)--O	-306.034		0	0	0	100	100
	29 (B2G)--O	-306.034		0	0	0	100	100
	30 (EU)--O	-305.993		0	0	0	100	100
	31 (EU)--O	-305.993		0	0	0	100	100
	32 (B1G)--O	-305.993		0	0	0	100	100
	33 (A1G)--O	-305.993		0	0	0	100	100
	34 (EU)--O	-305.981		0	0	0	100	100
	35 (EU)--O	-305.981		0	0	0	100	100
	36 B1G)--O	-305.981		0	0	0	100	100
	37 (A1G)--O	-305.981		0	0	0	100	100
	38 (A2G)--O	-305.963		0	0	0	100	100
	39 (EU)--O	-305.963		0	0	0	100	100
	40 (EU)--O	-305.963		0	0	0	100	100
	41 B2G)--O	-305.963		0	0	0	100	100

42 (A2G)--O	-305.955	0	0	0	100	100
43 (EU)--O	-305.955	0	0	0	100	100
44 (EU)--O	-305.955	0	0	0	100	100
45 (B2G)--O	-305.955	0	0	0	100	100
46 A1G)--O	-153.241	100	0	0	0	100
47 (A2U)--O	-104.532	100	0	0	0	100
48 (EU)--O	-104.416	100	0	0	0	100
49 (EU)--O	-104.416	100	0	0	0	100
50 (A1G)--O	-36.317	0.3	39.9	26.7	33.1	100
51 (EU)--O	-35.827	0.1	38.4	27.3	34.2	100
52 (EU)--O	-35.827	0.1	38.4	27.3	34.2	100
53 (B1G)--O	-34.825	0.3	60.6	0.8	38.3	100
54 (B2G)--O	-34.219	0	1.5	71.7	26.8	100
55 (EU)--O	-32.756	0.1	18.9	50.4	30.7	100
56 (EU)--O	-32.756	0.1	18.9	50.4	30.7	100
57 (A1G)--O	-31.699	0.1	13.2	46.6	40.2	100
58 (EU)--O	-31.268	0.1	17.1	1.6	81.2	100
59 (EU)--O	-31.268	0.1	17.1	1.6	81.2	100
60 (A1G)--O	-31.26	0.4	29.8	16	53.8	100
61 B1G)--O	-31.256	0.2	15	0	84.8	100
62 (A2G)--O	-28.462	0	2.1	5	92.9	100
63 (A1G)--O	-28.114	0.6	12.2	0.4	86.8	100
64 (EU)--O	-28.079	0.1	14.7	2.8	82.4	100
65 (EU)--O	-28.079	0.1	14.7	2.8	82.4	100
66 B1G)--O	-27.959	1	19.2	0.4	79.3	100
67 (EU)--O	-27.946	0	3.8	1.6	94.6	100
68 (EU)--O	-27.946	0	3.8	1.6	94.6	100
69 (B2G)--O	-27.855	0	0	1.8	98.2	100
70 (A2G)--O	-26.494	0	6.6	10.9	82.5	100
71 (EU)--O	-25.475	0	9	20	71	100
72 (EU)--O	-25.475	0	9	20	71	100
73 (B1G)--O	-23.711	10.7	16.1	10	63.1	100
74 (A1G)--O	-23.543	4.1	11.9	0.2	83.7	100
75 (EU)--O	-23.318	0.2	9.8	0.4	89.7	100
76 (EU)--O	-23.318	0.2	9.8	0.4	89.7	100
77 (B2G)--O	-23.229	0.3	3.4	11.3	85	100
78 (B1G)--O	-22.77	2.1	1.8	21.9	74.3	100
79 (EU)--O	-22.064	0	5.6	5.4	89	100
80 (EU)--O	-22.064	0	5.6	5.4	89	100
81 B2G)--O	-21.956	19	28.7	17.2	35.1	100
82 (A2G)--O	-21.76	0	6.9	3.1	89.9	100
83 (B1G)--O	-21.57	76.5	8.6	1.1	13.8	100
84 (A1G)--O	-21.064	69.2	10.1	0.4	20.3	100
85 (EG)--O	-20.856	98.3	1.5	0	0.2	100
86 (EG)--O	-20.856	98.3	1.5	0	0.2	100
87 (EU)--O	-20.244	0.1	18.8	9.3	71.8	100
88 (EU)--O	-20.244	0.1	18.8	9.3	71.8	100
89 (B2G)--O	-20.187	60.7	3	1	35.3	100
90 (A1G)--O	-20.166	42.8	2.5	1.3	53.4	100
91 (EU)--O	-19.604	0.2	22.8	24.3	52.8	100
92 (EU)--O	-19.604	0.2	22.8	24.3	52.8	100

93 (B1G)--O	-19.229	10	3.1	6.8	80.1	100
94 (B2G)--O	-18.669	6.4	3.8	5.1	84.7	100
95 (A2G)--O	-18.354	0	37.7	17.1	45.1	100
96 (EU)--O	-18.106	0	3	6.2	90.8	100
97 (EU)--O	-18.106	0	3	6.2	90.8	100
98 (A1G)--O	-17.752	10.3	15.9	0.4	73.4	100
99 (EU)--O	-17.492	0.4	13.8	0.5	85.3	100
100 (EU)--O	-17.492	0.4	13.8	0.5	85.3	100
101 A2G)--O	-17.489	0	0.1	11.4	88.5	100
102 (B1G)--O	-17.234	3.8	6.2	0.3	89.8	100
103 (A2U)--O	-16.928	0.3	30.7	19.9	49.1	100
104 (A1G)--O	-16.705	1	3.3	2.9	92.8	100
105 (EU)--O	-16.597	0	1.2	2	96.7	100
106 (EU)--O	-16.597	0	1.2	2	96.7	100
107 (B2G)--O	-16.581	0	0	1.7	98.3	100
108 (EG)--O	-16.268	2.4	26.5	18.4	52.7	100
109 (EG)--O	-16.268	2.4	26.5	18.4	52.7	100
110 (A2G)--O	-16.201	0	0.5	4.7	94.9	100
111 (EU)--O	-16.13	0.2	7.2	5	87.6	100
112 (EU)--O	-16.13	0.2	7.2	5	87.6	100
113 (B1G)--O	-15.866	2.6	4.3	5.3	87.8	100
114 (A1G)--O	-15.303	12.2	32.4	11.3	44.2	100
115 (B2U)--O	-15.264	0	32.5	0	67.5	100
116 B2G)--O	-14.348	0	0	3.1	96.9	100
117 (EU)--O	-14.269	0.3	6.8	7.2	85.6	100
118 (EU)--O	-14.269	0.3	6.8	7.2	85.6	100
119 (B1U)--O	-13.988	0	0.1	56.7	43.3	100
120 (A2G)--O	-13.954	0	2.1	1.4	96.5	100
121 (EU)--O	-13.94	1.9	37.3	4.2	56.6	100
122 (EU)--O	-13.94	1.9	37.3	4.2	56.6	100
123 (A1G)--O	-13.761	0	2	6.2	91.8	100
124 (A2U)--O	-13.417	0.2	9.5	3.2	87.1	100
125 (EG)--O	-13.416	0.2	5.1	11.5	83.1	100
126 (EG)--O	-13.416	0.2	5.1	11.5	83.1	100
127 (B1G)--O	-13.376	1.1	3.9	2.6	92.4	100
128 (EU)--O	-13.326	0.6	11.3	8.6	79.5	100
129 (EU)--O	-13.326	0.6	11.3	8.6	79.5	100
130 (B2U)--O	-12.854	0	34	0	66	100
131 A1G)--O	-12.848	0.5	14.4	56.5	28.7	100
132 (EU)--O	-11.809	0.3	21.3	49.8	28.7	100
133 (EU)--O	-11.809	0.3	21.3	49.8	28.7	100
134 (EG)--O	-11.601	0.6	29.2	27.4	42.7	100
135 (EG)--O	-11.601	0.6	29.2	27.4	42.7	100
136 B2G)--O	-11.274	0.3	13.8	63.1	22.7	100
137 (B1G)--O	-10.991	10.7	63.4	1.2	24.7	100
138 (A1U)--O	-9.845	0	0	0	100	100
139 (A2U)--O	-9.562	1.5	47.8	23.5	27.3	100
140 (B1U)--O	-9.222	0	0	4.9	95.1	100
141 (EG)--O	-9.175	0.1	4.7	10.2	85	100
142 (EG)--O	-9.175	0.1	4.7	10.2	85	100
143 (EG)--O	-9.065	0.4	20.7	0	78.9	100

144 (EG)--O	-9.065	0.4	20.7	0	78.9	100
145 (B2U)--O	-8.987	0	22.7	0	77.3	100
146 A2U)--O	-8.813	0.1	5.5	36.1	58.3	100
147 (A1U)--O	-5.048	0	0.1	0.2	99.7	100
148 (EG)--V	-0.119	0.1	12.2	16.1	71.5	100
149 (EG)--V	-0.119	0.1	12.2	16.1	71.5	100
150 (B1U)--V	2.51	0	0	18.6	81.4	100
151 A2U)--V	2.834	45.5	0.7	4.1	49.8	100
152 (B2U)--V	2.884	0	16.3	0	83.7	100
153 (EG)--V	3.295	0	4.2	3	92.8	100
154 (EG)--V	3.295	0	4.2	3	92.8	100
155 (A2U)--V	3.775	50.3	7.9	0.3	41.4	100
156 A1G)--V	3.839	86.5	5.7	0.2	7.6	100
157 (A1U)--V	4.924	0	0	0	99.9	100
158 (EG)--V	5.061	0	1.9	1.2	97	100
159 (EG)--V	5.061	0	1.9	1.2	97	100
160 (EU)--V	5.343	76.5	3	1.1	19.3	100
161 (EU)--V	5.343	76.5	3	1.1	19.3	100
162 (B2U)--V	6.019	0	19.3	0.1	80.6	100
163 (B1U)--V	6.477	0	0.1	20.9	79.1	100
164 (A1G)--V	6.52	0.3	0	0.9	98.8	100
165 (EU)--V	6.641	0.5	0	0.2	99.2	100
166 (EU)--V	6.641	0.5	0	0.2	99.2	100
167 (B1G)--V	6.763	0	0	0.1	99.9	100
168 (B2G)--V	7.546	0	0.5	0.1	99.4	100
169 (EU)--V	7.829	0	0.7	0.4	98.9	100
170 (EU)--V	7.829	0	0.7	0.4	98.9	100
171 A2U)--V	8.109	52.3	5.8	12.1	29.8	100
172 (A2G)--V	8.199	0	0.5	0.1	99.4	100
173 (A1G)--V	8.218	2.2	0.1	5.4	92.3	100
174 (EG)--V	8.415	0.1	13.6	15.7	70.6	100
175 (EG)--V	8.415	0.1	13.6	15.7	70.6	100
176 (EU)--V	8.521	0.2	0	1.7	98.1	100
177 (EU)--V	8.521	0.2	0	1.7	98.1	100
178 (B2G)--V	8.558	0	0	2.3	97.7	100
179 (EU)--V	9.125	0	0.5	0.1	99.4	100
180 (EU)--V	9.125	0	0.5	0.1	99.4	100
181 B1G)--V	9.156	0	1.5	0	98.5	100
182 (A2G)--V	9.174	0	0	0	100	100
183 (A1G)--V	9.571	47.3	2.8	4.4	45.5	100
184 (A1U)--V	10.509	0	0	0	100	100
185 (B2G)--V	10.529	0.1	1.4	23.7	74.8	100
186 (EU)--V	10.611	3	9.7	8.7	78.6	100
187 (EU)--V	10.611	3	9.7	8.7	78.6	100
188 (B1U)--V	10.673	0	0	4.5	95.5	100
189 (EG)--V	10.728	0	1	4.4	94.6	100
190 (EG)--V	10.728	0	1	4.4	94.6	100
191 A1G)--V	11.178	0.4	0.8	3.9	94.9	100
192 (B1G)--V	11.496	0	31.6	1.5	67	100
193 (A2G)--V	11.651	0	4.1	0.2	95.7	100
194 (EU)--V	11.749	0.3	0.4	0.8	98.5	100



195 (EU)--V	11.749	0.3	0.4	0.8	98.5	100
196 B2G)--V	11.82	0	0.5	8.5	90.9	100
197 (A2U)--V	11.825	56.2	10.6	7	26.2	100
198 (EU)--V	11.952	0.2	1.3	5.4	93.1	100
199 (EU)--V	11.952	0.2	1.3	5.4	93.1	100
200 (A2G)--V	12.123	0	0.2	0.1	99.7	100
201 B1G)--V	12.431	0	0.7	0.2	99	100
202 (EU)--V	12.695	0.6	1.1	1.1	97.2	100
203 (EU)--V	12.695	0.6	1.1	1.1	97.2	100
204 (A1G)--V	12.949	0.7	2.3	10.5	86.5	100
205 (A1G)--V	13.253	8.3	2.3	18.9	70.5	100
206 (EU)--V	13.517	0.3	11.7	5.2	82.8	100
207 (EU)--V	13.517	0.3	11.7	5.2	82.8	100
208 (B1G)--V	13.907	0	0.5	0.4	99.1	100
209 (EU)--V	14.291	0.4	3.9	20.5	75.2	100
210 (EU)--V	14.291	0.4	3.9	20.5	75.2	100
211 B2G)--V	14.338	0	1.9	5.2	92.8	100
212 (A1G)--V	14.409	0.4	6	2.8	90.7	100
213 (B2G)--V	14.602	0	2.8	24.4	72.8	100
214 (EU)--V	14.718	1.2	4.4	0.6	93.8	100
215 (EU)--V	14.718	1.2	4.4	0.6	93.8	100
216 B1G)--V	15.185	0	6.6	0	93.4	100
217 (A1G)--V	15.862	1.5	21.4	10.2	66.9	100
218 (EU)--V	15.904	2	3.4	14.5	80.1	100
219 (EU)--V	15.904	2	3.4	14.5	80.1	100
220 (B2G)--V	15.941	0	4.4	7.5	88.1	100
221 B1G)--V	16.808	0	19.3	11.1	69.6	100
222 (A2G)--V	17.051	0	4.9	8.1	87	100
223 (EU)--V	17.277	1.3	8.6	12.2	77.9	100
224 (EU)--V	17.277	1.3	8.6	12.2	77.9	100
225 (A2G)--V	17.666	0	0.4	2.6	97	100
226 (EU)--V	17.917	0.8	1.4	2.9	94.9	100
227 (EU)--V	17.917	0.8	1.4	2.9	94.9	100
228 (EU)--V	19.714	1.6	2.4	2.5	93.4	100
229 (EU)--V	19.714	1.6	2.4	2.5	93.4	100
230 (B1G)--V	19.923	0	34	5.1	60.8	100
231 (EG)--V	19.942	0	1.2	1.1	97.7	100
232 (EG)--V	19.942	0	1.2	1.1	97.7	100
233 (A2G)--V	20.178	0	0.1	4.7	95.2	100
234 (B2U)--V	20.179	0	0.4	0	99.5	100
235 (B2G)--V	20.198	0	0.3	0	99.7	100
236 A1G)--V	20.269	0.5	4	2.5	93	100
237 (A2U)--V	20.274	3.2	0.3	0.6	95.9	100
238 (EU)--V	20.802	0.3	2.7	3	93.9	100
239 (EU)--V	20.802	0.3	2.7	3	93.9	100
240 (EG)--V	20.9	0	1.5	1.4	97.2	100
241 (EG)--V	20.9	0	1.5	1.4	97.2	100
242 (B1G)--V	20.977	0	7.7	0.4	91.9	100
243 (A2G)--V	21.051	0	1.4	4.5	94.1	100
244 (EU)--V	21.058	0.2	1.1	2	96.7	100
245 (EU)--V	21.058	0.2	1.1	2	96.7	100

246 B1U)--V	21.157	0	0	3.5	96.5	100
247 (EU)--V	21.59	0.1	0.4	0.7	98.7	100
248 (EU)--V	21.59	0.1	0.4	0.7	98.7	100
249 (A1G)--V	21.628	1.4	1.7	5.1	91.7	100
250 (B2G)--V	21.706	0	0.4	1	98.6	100
251 B2U)--V	21.731	0	1.2	0.1	98.7	100
252 (A2U)--V	21.757	6.8	1.5	1.2	90.5	100
253 (EU)--V	21.894	0.1	1.2	0.7	98	100
254 (EU)--V	21.894	0.1	1.2	0.7	98	100
255 (A2G)--V	21.935	0	0.2	0.4	99.5	100
256 (EG)--V	22.012	0	0.4	1.1	98.5	100
257 (EG)--V	22.012	0	0.4	1.1	98.5	100
258 (B2G)--V	22.05	0	1.4	1.4	97.2	100
259 (B1G)--V	22.082	0	21.5	1.6	76.9	100
260 (A1U)--V	22.126	0	0	0	100	100
261 A1G)--V	22.182	0.7	21.6	6.4	71.3	100
262 (EU)--V	22.708	0.9	21.2	5.8	72.2	100
263 (EU)--V	22.708	0.9	21.2	5.8	72.2	100
264 (A1G)--V	22.845	0.3	15.3	16.1	68.3	100
265 (B2G)--V	22.854	0	1.7	0.8	97.5	100
266 (EU)--V	22.87	1.5	15.1	3	80.3	100
267 (EU)--V	22.87	1.5	15.1	3	80.3	100
268 (A2G)--V	22.875	0	0.6	1.3	98	100
269 (B1G)--V	22.955	0	9.9	1.9	88.2	100
270 (B1U)--V	23.014	0	0	1.1	98.9	100
271 (EU)--V	23.062	0.5	15.1	5.8	78.6	100
272 (EU)--V	23.062	0.5	15.1	5.8	78.6	100
273 (EG)--V	23.336	0	2.4	0.8	96.8	100
274 (EG)--V	23.336	0	2.4	0.8	96.8	100
275 (A1G)--V	23.9	1.7	2.4	22.1	73.9	100
276 A2U)--V	24.16	2.3	1	1.2	95.6	100
277 (EG)--V	24.281	0	0.8	2.6	96.6	100
278 (EG)--V	24.281	0	0.8	2.6	96.6	100
279 (A2G)--V	24.398	0	1.5	4.3	94.2	100
280 (A1U)--V	24.402	0	0	0	100	100
281 B2U)--V	24.421	0	1.1	0	98.8	100
282 (EU)--V	24.552	2	3.7	3.2	91.1	100
283 (EU)--V	24.552	2	3.7	3.2	91.1	100
284 (EU)--V	25.127	0.7	0.9	15.5	82.9	100
285 (EU)--V	25.127	0.7	0.9	15.5	82.9	100
286 B1U)--V	25.232	0	0	2.1	97.9	100
287 (B2G)--V	25.286	0	0.4	14.2	85.3	100
288 (EG)--V	25.328	0	0.3	0.3	99.4	100
289 (EG)--V	25.328	0	0.3	0.3	99.4	100
290 (A2U)--V	25.492	0.3	0.3	2	97.4	100
291 B1G)--V	26.253	0.1	7.7	10.3	81.9	100
292 (A1G)--V	26.357	4.6	20.2	4	71.3	100
293 (B2U)--V	26.638	0	0.8	0	99.2	100
294 (EG)--V	26.81	0	0.4	0.7	98.9	100
295 (EG)--V	26.81	0	0.4	0.7	98.9	100
296 A1U)--V	26.967	0	0	0	100	100

297 (EU)--V	27.454	3.5	10	6.1	80.4	100
298 (EU)--V	27.454	3.5	10	6.1	80.4	100
299 (B1U)--V	27.705	0	0	2.8	97.2	100
300 (EG)--V	28.527	0.1	17.4	4.3	78.2	100
301 (EG)--V	28.527	0.1	17.4	4.3	78.2	100
302 (B2G)--V	28.839	0	1.2	5.3	93.5	100
303 (EU)--V	29.119	0.2	2.1	2.2	95.5	100
304 (EU)--V	29.119	0.2	2.1	2.2	95.5	100
305 (A1G)--V	29.129	0.2	2.3	3.4	94.1	100
306 (EG)--V	29.503	0.1	10.8	2.3	86.8	100
307 (EG)--V	29.503	0.1	10.8	2.3	86.8	100
308 (A2U)--V	29.647	1	11.3	63.1	24.7	100
309 (B2G)--V	29.648	0	1.6	1.3	97.1	100
310 (A2G)--V	29.728	0	1.2	1.1	97.7	100
311 (EU)--V	29.789	0.1	0.1	0.7	99.1	100
312 (EU)--V	29.789	0.1	0.1	0.7	99.1	100
313 (A2G)--V	29.903	0	2.1	1.3	96.6	100
314 (A1G)--V	29.961	0.5	9.9	6.6	83	100
315 (B2G)--V	30.134	0	0	11.9	88	100
316 (EU)--V	30.264	0.1	1.6	0.5	97.8	100
317 (EU)--V	30.264	0.1	1.6	0.5	97.8	100
318 (B1G)--V	30.305	0	3.3	2	94.7	100
319 (EU)--V	30.325	0	3.6	3.4	93	100
320 (EU)--V	30.325	0	3.6	3.4	93	100
321 (A1U)--V	30.84	0	0	0	100	100
322 (B1G)--V	30.952	0	0.7	0.7	98.6	100
323 (EU)--V	30.989	0.2	1.5	3.5	94.8	100
324 (EU)--V	30.989	0.2	1.5	3.5	94.8	100
325 (A1G)--V	31.036	1.8	1.9	21.3	75	100
326 (B2G)--V	31.24	0	6.9	5.2	87.9	100
327 (A2G)--V	31.43	0	0.1	4.5	95.3	100
328 (B1G)--V	31.633	0	19.2	13.9	66.9	100
329 (B2U)--V	31.71	0	72.8	0	27.2	100
330 (A1G)--V	31.867	0.7	9.8	5.9	83.7	100
331 (EG)--V	32.138	0.1	15.5	43.3	41.1	100
332 (EG)--V	32.138	0.1	15.5	43.3	41.1	100
333 (EU)--V	32.14	0.1	9.6	6.3	84	100
334 (EU)--V	32.14	0.1	9.6	6.3	84	100
335 (B1U)--V	32.177	0	0	66.9	33.1	100
336 (EU)--V	32.395	0.3	2.4	2	95.3	100
337 (EU)--V	32.395	0.3	2.4	2	95.3	100
338 (A2G)--V	32.551	0	0.1	0.3	99.6	100
339 (B1G)--V	32.557	0	0.5	0.1	99.4	100
340 (EU)--V	33.127	0.6	0.6	7.2	91.5	100
341 (EU)--V	33.127	0.6	0.6	7.2	91.5	100
342 (B2G)--V	33.588	0	1.6	3.1	95.4	100
343 (EU)--V	33.819	0.2	5.4	4.8	89.6	100
344 (EU)--V	33.819	0.2	5.4	4.8	89.6	100
345 (B1G)--V	33.849	0	6.1	3.2	90.7	100
346 (B2G)--V	34.364	0	0	0.8	99.2	100
347 (A2U)--V	34.398	4.6	45.7	15.7	33.9	100

348 (EU)--V	34.432	0	4.1	3.7	92.2	100
349 (EU)--V	34.432	0	4.1	3.7	92.2	100
350 (A2G)--V	34.604	0	0	1.8	98.1	100
351 A1G)--V	34.691	0.1	4	3.6	92.3	100
352 (EU)--V	34.842	0	0.8	3.1	96.2	100
353 (EU)--V	34.842	0	0.8	3.1	96.2	100
354 (A1G)--V	34.984	0.1	3.2	7	89.8	100
355 (B2G)--V	35.393	0	8.4	4.3	87.3	100
356 A2G)--V	35.692	0	0.6	0.5	98.9	100
357 (EU)--V	36.006	0	4.3	4.2	91.5	100
358 (EU)--V	36.006	0	4.3	4.2	91.5	100
359 (A2G)--V	37.231	0	4.3	4.7	91	100
360 (EU)--V	37.43	0	0.6	1.8	97.6	100
361 (EU)--V	37.43	0	0.6	1.8	97.6	100
362 (B1G)--V	37.732	0	4.9	0.9	94.2	100
363 (B1G)--V	37.765	0	2.9	14.2	82.9	100
364 (B2G)--V	37.806	0	0.7	3.1	96.2	100
365 (EU)--V	38.299	0.1	5.5	5.4	89	100
366 (EU)--V	38.299	0.1	5.5	5.4	89	100
367 (A1G)--V	38.341	0.5	5.1	3.8	90.7	100
368 (B2G)--V	38.709	0	3.1	5.8	91.1	100
369 (A1G)--V	39.665	4.2	2.9	0.5	92.4	100
370 (B2U)--V	39.725	0	7.4	7.9	84.6	100
371 (EU)--V	39.868	0.7	2.8	5.5	90.9	100
372 (EU)--V	39.868	0.7	2.8	5.5	90.9	100
373 (A2G)--V	40.14	0	0.5	14.6	84.9	100
374 (EG)--V	40.166	0.1	5.5	13.6	80.8	100
375 (EG)--V	40.166	0.1	5.5	13.6	80.8	100
376 (EU)--V	40.504	0.3	3.6	10.4	85.6	100
377 (EU)--V	40.504	0.3	3.6	10.4	85.6	100
378 (A2U)--V	40.823	0.2	1.1	11	87.7	100
379 (B2G)--V	41.079	0	1.8	1.6	96.7	100
380 (EU)--V	41.829	0.1	1.6	9.7	88.6	100
381 (EU)--V	41.829	0.1	1.6	9.7	88.6	100
382 (A2G)--V	41.859	0	1.2	9.6	89.2	100
383 (B1G)--V	41.883	0.5	26	5.6	67.9	100
384 (EG)--V	41.9	0	9.3	9	81.7	100
385 (EG)--V	41.9	0	9.3	9	81.7	100
386 A1U)--V	41.906	0	19.9	17	63.1	100
387 (B2U)--V	42.001	0	7.8	9.2	83	100
388 (B1U)--V	42.957	0	5.4	8	86.6	100
389 (B1G)--V	43.049	0	0.7	4	95.3	100
390 (EG)--V	43.095	0.1	5.3	8.4	86.2	100
391 (EG)--V	43.095	0.1	5.3	8.4	86.2	100
392 (A1U)--V	43.368	0	3.1	6.4	90.5	100
393 (A2U)--V	43.704	4.4	29	15.7	50.9	100
394 (EG)--V	43.995	1.5	18.5	7.7	72.2	100
395 (EG)--V	43.995	1.5	18.5	7.7	72.2	100
396 B1G)--V	44.067	0	5.8	0.2	94	100
397 (EU)--V	44.199	0.1	2.3	0.8	96.8	100
398 (EU)--V	44.199	0.1	2.3	0.8	96.8	100

399 (A1G)--V	44.289	3.6	6.7	0.1	89.6	100
400 (EU)--V	44.625	0.3	6.6	0.1	93	100
401 (EU)--V	44.625	0.3	6.6	0.1	93	100
402 (B2U)--V	45.672	0	27	0.8	72.2	100
403 (A1G)--V	45.674	0.4	1.2	0	98.4	100
404 (B2G)--V	45.725	0	0	0.6	99.4	100
405 (EU)--V	45.912	0	0.9	2.1	97	100
406 (EU)--V	45.912	0	0.9	2.1	97	100
407 (A2G)--V	45.914	0	2.4	17.9	79.7	100
408 (B1G)--V	45.991	0	0.2	1.5	98.3	100
409 (EG)--V	46.719	0.1	3.3	4.8	91.8	100
410 (EG)--V	46.719	0.1	3.3	4.8	91.8	100
411 A2U)--V	46.724	0.5	1.7	2.3	95.5	100
412 (B2U)--V	46.802	0	0.1	0.6	99.3	100
413 (EG)--V	47.103	0.3	12.2	11.1	76.3	100
414 (EG)--V	47.103	0.3	12.2	11.1	76.3	100
415 (A2U)--V	47.31	2.4	10.3	1.1	86.2	100
416 (EU)--V	47.722	0	1.5	1.3	97.2	100
417 (EU)--V	47.722	0	1.5	1.3	97.2	100
418 (B2U)--V	47.78	0	2.5	0.8	96.7	100
419 (B1U)--V	47.781	0	17.9	21.5	60.6	100
420 (EG)--V	48.068	0.1	2.8	1.2	95.9	100
421 (EG)--V	48.068	0.1	2.8	1.2	95.9	100
422 (A1U)--V	48.094	0	0	0	100	100
423 (B1U)--V	48.176	0	5.1	6.6	88.3	100
424 (EG)--V	48.255	0.6	18.5	9.6	71.3	100
425 (EG)--V	48.255	0.6	18.5	9.6	71.3	100
426 A2G)--V	48.369	0	4.2	0.1	95.7	100
427 (A2U)--V	49.135	7.3	36.7	6.7	49.3	100
428 (A2G)--V	49.73	0	3.9	5	91.1	100
429 (EU)--V	50.666	0.7	18.7	1.2	79.5	100
430 (EU)--V	50.666	0.7	18.7	1.2	79.5	100
431 B2G)--V	50.798	0	0.1	1.3	98.6	100
432 (A1G)--V	50.829	0.1	47.1	0.7	52.1	100
433 (EU)--V	51.03	0.2	3.9	1.4	94.6	100
434 (EU)--V	51.03	0.2	3.9	1.4	94.6	100
435 (B1G)--V	52.303	0	38.8	3.2	57.9	100
436 A1G)--V	52.719	1.4	26	15.5	57.1	100
437 (B2G)--V	53.26	0	0.2	22.9	76.9	100
438 (EU)--V	54.52	0.5	0.8	46.2	52.5	100
439 (EU)--V	54.52	0.5	0.8	46.2	52.5	100
440 (A1G)--V	54.875	1	1.9	57.9	39.2	100
441 B1G)--V	55.597	0	41.7	10.7	47.5	100
442 (EU)--V	55.738	0.2	25.4	3.5	70.9	100
443 (EU)--V	55.738	0.2	25.4	3.5	70.9	100
444 (B1U)--V	55.757	0	1.4	13.2	85.5	100
445 (A1G)--V	55.925	0.5	42	3.2	54.2	100
446 (EG)--V	56.094	0	2.4	10.5	87	100
447 (EG)--V	56.094	0	2.4	10.5	87	100
448 (A1U)--V	56.613	0	3.6	2.8	93.6	100
449 (B2G)--V	57.244	0	0	2.3	97.6	100

450 (B1G)--V	57.339	0	50.7	1.3	48	100
451 (EU)--V	57.718	0.1	0.2	8.9	90.8	100
452 (EU)--V	57.718	0.1	0.2	8.9	90.8	100
453 (A1G)--V	57.965	0.2	4.3	22.6	73	100
454 (EU)--V	58.028	0.1	18.6	7.3	74	100
455 (EU)--V	58.028	0.1	18.6	7.3	74	100
456 A2G)--V	58.038	0	0.4	0	99.6	100
457 (A2U)--V	58.199	0.4	10.5	25.7	63.4	100
458 (A1G)--V	58.664	0.4	22.6	30.9	46.1	100
459 (EU)--V	58.874	0	1	1.2	97.8	100
460 (EU)--V	58.874	0	1	1.2	97.8	100
461 B1G)--V	59.213	0	30.4	5.3	64.2	100
462 (B2G)--V	59.406	0	0.1	2.2	97.8	100
463 (EG)--V	59.446	0.3	15.6	17.7	66.4	100
464 (EG)--V	59.446	0.3	15.6	17.7	66.4	100
465 (A2G)--V	59.53	0	0.4	0	99.6	100
466 (EU)--V	59.674	0	2.5	2.7	94.9	100
467 (EU)--V	59.674	0	2.5	2.7	94.9	100
468 (A1G)--V	60.578	0.1	9.8	32.6	57.6	100
469 (B2U)--V	60.667	0	24.8	10.6	64.5	100
470 (B1G)--V	60.698	0	11.5	5.1	83.4	100
471 (EU)--V	60.976	1.1	5.4	11.3	82.3	100
472 (EU)--V	60.976	1.1	5.4	11.3	82.3	100
473 (B1G)--V	61.322	0	1	0.2	98.8	100
474 (EU)--V	61.523	0.7	11.8	7.4	80.2	100
475 (EU)--V	61.523	0.7	11.8	7.4	80.2	100
476 A2G)--V	61.984	0	0.1	0.7	99.3	100
477 (EU)--V	62.045	17.1	30.5	1.7	50.8	100
478 (EU)--V	62.045	17.1	30.5	1.7	50.8	100
479 (A1G)--V	62.381	0.6	6.4	9.6	83.4	100
480 (B2G)--V	62.988	0	0.4	7	92.6	100
481 B2U)--V	63.003	0	29.6	15.8	54.6	100
482 (EU)--V	63.171	0	1.6	0.5	97.9	100
483 (EU)--V	63.171	0	1.6	0.5	97.9	100
484 (EU)--V	64.173	0.4	14.4	7.2	78.1	100
485 (EU)--V	64.173	0.4	14.4	7.2	78.1	100
486 A1G)--V	64.281	0.1	19.3	13.8	66.8	100
487 (EG)--V	64.385	0.6	27.9	19	52.5	100
488 (EG)--V	64.385	0.6	27.9	19	52.5	100
489 (B1G)--V	64.658	0	29.3	4.4	66.3	100
490 (A2G)--V	65.274	0	7.4	4.6	88.1	100
491 B1U)--V	65.514	0	2.2	28.7	69.1	100
492 (A2U)--V	65.581	0.3	4.4	20.9	74.3	100
493 (EG)--V	65.662	1	6.2	19.3	73.5	100
494 (EG)--V	65.662	1	6.2	19.3	73.5	100
495 (A1U)--V	65.748	0	24.1	10.4	65.5	100
496 B2G)--V	65.886	0	0.2	0.1	99.7	100
497 (EU)--V	66.19	0	2.3	4.7	92.9	100
498 (EU)--V	66.19	0	2.3	4.7	92.9	100
499 (EU)--V	66.26	0.1	0.7	0.9	98.3	100
500 (EU)--V	66.26	0.1	0.7	0.9	98.3	100

501 A2G)--V	66.626	0	1.8	1.9	96.3	100
502 (B1G)--V	66.955	0	3.6	8.1	88.3	100
503 (B2G)--V	67.005	0	0.6	9.1	90.4	100
504 (EU)--V	67.413	0.2	1.2	4.4	94.2	100
505 (EU)--V	67.413	0.2	1.2	4.4	94.2	100
506 A1G)--V	67.785	1	5.5	0.9	92.6	100
507 (EG)--V	68.077	2	11.8	3.7	82.4	100
508 (EG)--V	68.077	2	11.8	3.7	82.4	100
509 (B1U)--V	68.318	0	9	13.2	77.8	100
510 (A1U)--V	69.242	0	6.8	5.4	87.8	100
511 A2G)--V	69.274	0	0.4	1.9	97.6	100
512 (B2U)--V	69.346	0	1	0	99	100
513 (EU)--V	69.671	0.1	5.7	9.4	84.9	100
514 (EU)--V	69.671	0.1	5.7	9.4	84.9	100
515 (EG)--V	69.961	2.1	9.1	0.3	88.6	100
516 (EG)--V	69.961	2.1	9.1	0.3	88.6	100
517 (B1U)--V	70.079	0	7.2	1.4	91.5	100
518 (EG)--V	70.141	8	2.1	4.6	85.3	100
519 (EG)--V	70.141	8	2.1	4.6	85.3	100
520 (A2U)--V	70.392	0.2	30.9	6.6	62.3	100
521 A2U)--V	70.507	0.1	11.7	0.8	87.4	100
522 (A1U)--V	70.639	0	0.1	5.2	94.7	100
523 (B2G)--V	70.858	0	0.3	9.2	90.6	100
524 (EG)--V	71.077	65	10.3	3.3	21.4	100
525 (EG)--V	71.077	65	10.3	3.3	21.4	100
526 A2G)--V	71.279	0	4.5	1.5	94	100
527 (EU)--V	71.458	2.1	12.2	9.8	75.9	100
528 (EU)--V	71.458	2.1	12.2	9.8	75.9	100
529 (B2U)--V	71.556	0	2.2	1.2	96.6	100
530 (B1G)--V	71.582	0	35.2	16.2	48.6	100
531 (EG)--V	71.611	1.7	7.3	4.1	86.8	100
532 (EG)--V	71.611	1.7	7.3	4.1	86.8	100
533 (A1G)--V	71.92	0.2	1.4	17.5	81	100
534 (EU)--V	73.4	0.2	2.5	29.4	67.9	100
535 (EU)--V	73.4	0.2	2.5	29.4	67.9	100
536 B1U)--V	73.59	0	18.6	1.7	79.7	100
537 (A2G)--V	74.086	0	0.1	0.1	99.9	100
538 (B2G)--V	74.432	0.1	2.2	37.1	60.6	100
539 (EU)--V	74.532	0	0.2	0.9	98.8	100
540 (EU)--V	74.532	0	0.2	0.9	98.8	100
541 (EG)--V	74.703	2.2	16.2	8.4	73.1	100
542 (EG)--V	74.703	2.2	16.2	8.4	73.1	100
543 (B2G)--V	74.795	0.2	1	13	85.8	100
544 (B1G)--V	74.855	0	2.5	0.1	97.4	100
545 (B2G)--V	76.632	2.2	8.7	18.5	70.6	100
546 A1U)--V	76.908	0	3	6.8	90.2	100
547 (A2U)--V	77.085	0.2	9.3	18.6	71.9	100
548 (EU)--V	77.212	0.2	8.5	13.5	77.8	100
549 (EU)--V	77.212	0.2	8.5	13.5	77.8	100
550 (A1G)--V	77.289	1.1	13.4	0.8	84.7	100
551 (EG)--V	78.224	0	8.1	10	81.8	100

552 (EG)--V	78.224	0	8.1	10	81.8	100
553 (A1U)--V	79.433	0	13.2	12	74.8	100
554 (B1U)--V	79.514	0	13.1	8.4	78.6	100
555 (A2G)--V	80.645	0	0.3	0.1	99.6	100
556 (EU)--V	80.872	0	0.1	0.2	99.7	100
557 (EU)--V	80.872	0	0.1	0.2	99.7	100
558 (A1G)--V	80.898	2.2	23.5	33.3	41	100
559 (B2G)--V	81.143	0.1	0.4	0.1	99.5	100
560 (B1G)--V	81.305	0.4	58	3.8	37.8	100
561 (EG)--V	81.407	0.6	6.5	9.9	83	100
562 (EG)--V	81.407	0.6	6.5	9.9	83	100
563 (EU)--V	81.907	0.1	16.8	7.4	75.8	100
564 (EU)--V	81.907	0.1	16.8	7.4	75.8	100
565 (B1G)--V	82.024	0	1.1	0.1	98.7	100
566 B1U)--V	82.23	0	0.2	4.1	95.7	100
567 (A1G)--V	82.407	0.7	16.7	26.6	56.1	100
568 (EU)--V	82.408	0.1	26.4	19.9	53.6	100
569 (EU)--V	82.408	0.1	26.4	19.9	53.6	100
570 (A2G)--V	82.427	0	7.2	4.3	88.5	100
571 (EU)--V	82.546	0	7.1	16	76.9	100
572 (EU)--V	82.546	0	7.1	16	76.9	100
573 (B1G)--V	82.68	0.1	32	11.9	56.1	100
574 (B2U)--V	83.549	0	15.6	31.3	53	100
575 (A1U)--V	83.638	0	5.8	17.5	76.7	100
576 (EG)--V	83.74	0.4	10.5	23.2	65.9	100
577 (EG)--V	83.74	0.4	10.5	23.2	65.9	100
578 (EU)--V	83.779	0.1	46.9	10.6	42.4	100
579 (EU)--V	83.779	0.1	46.9	10.6	42.4	100
580 (A1G)--V	83.839	1.2	44.3	15.1	39.5	100
581 B1G)--V	83.86	0.1	36.3	5.6	58	100
582 (A1G)--V	84.827	10.2	28.8	2	59	100
583 (B2G)--V	84.866	0.1	0.4	6.5	93	100
584 (EU)--V	85.49	0	0.6	4.9	94.5	100
585 (EU)--V	85.49	0	0.6	4.9	94.5	100
586 B2G)--V	85.523	0.2	5.8	17.8	76.3	100
587 (A2G)--V	86.106	0	0.2	4.9	94.8	100
588 (B2G)--V	86.784	0	0	1.5	98.4	100
589 (B1G)--V	86.929	2.8	39.8	2.2	55.2	100
590 (EU)--V	87.452	0	5.9	4.6	89.6	100
591 (EU)--V	87.452	0	5.9	4.6	89.6	100
592 (EU)--V	88.472	0.1	7.5	3.3	89.1	100
593 (EU)--V	88.472	0.1	7.5	3.3	89.1	100
594 (A2G)--V	88.845	0	1.3	1.5	97.2	100
595 (A1G)--V	88.956	0.3	22.1	25.4	52.2	100
596 (EU)--V	89.506	0.3	5.8	10.4	83.5	100
597 (EU)--V	89.506	0.3	5.8	10.4	83.5	100
598 (B2G)--V	90.474	0	0.2	9.7	90.1	100
599 (A2G)--V	91.249	0	0.1	0.2	99.7	100
600 (B1G)--V	92.16	1.3	8.1	7.6	83	100
601 (EU)--V	92.495	0.1	12.1	11.2	76.6	100
602 (EU)--V	92.495	0.1	12.1	11.2	76.6	100



603 (A1G)--V	93.08	1.2	4.8	7.4	86.6	100
604 (A2G)--V	93.666	0	22.2	6.5	71.4	100
605 (B2G)--V	95.025	0	2.4	2.8	94.8	100
606 (EU)--V	95.407	0	1.7	7.8	90.5	100
607 (EU)--V	95.407	0	1.7	7.8	90.5	100
608 (EU)--V	97.901	0.2	6.5	20.2	73.1	100
609 (EU)--V	97.901	0.2	6.5	20.2	73.1	100
610 (B1G)--V	99.803	1.6	5.9	27	65.5	100
611 A1G)--V	101.494	0.6	3.4	55.8	40.2	100
612 (B2G)--V	101.638	0	1	2.1	96.9	100
613 (EU)--V	102.936	0	1.4	3.2	95.4	100
614 (EU)--V	102.936	0	1.4	3.2	95.4	100
615 (A2G)--V	103.687	0	2.1	5.4	92.5	100
616 A2G)--V	103.849	0	5.8	7.2	87	100
617 (EU)--V	105.89	0	6.1	5.1	88.7	100
618 (EU)--V	105.89	0	6.1	5.1	88.7	100
619 (B2G)--V	106.592	0	4.4	3.7	92	100

**Supporting Information Table 3.** Calculated molecular orbital energies and compositions of PcZn using selected exchange-correlation functionals and molecular geometry optimized in gas-phase using B3LYP exchange-correlation functional.<sup>a</sup>

orbital	symmetry	E, (eV)	Zn	N <sub>pyrr</sub>	N <sub>meso</sub>	C(Pc)
BP86						
154	e <sub>g</sub>	-1.382	0.1	26	26.1	86.5
153	e <sub>g</sub>	-1.382	0.1	26	26.1	86.5
151	b <sub>2u</sub>	-1.651	0	37.8	37.8	65.2
150	b <sub>1u</sub>	-1.87	0	73.4	73.4	62.7
<b>149</b>	<b>e<sub>g</sub></b>	<b>-3.291</b>	<b>0.4</b>	<b>84.1</b>	<b>84.6</b>	<b>27.6</b>
<b>148</b>	<b>e<sub>g</sub></b>	<b>-3.291</b>	<b>0.4</b>	<b>84.1</b>	<b>84.6</b>	<b>27.6</b>
<b>147</b>	<b>a<sub>1u</sub></b>	<b>-4.746</b>	<b>0</b>	<b>67.8</b>	<b>67.8</b>	<b>36</b>
146	b <sub>1g</sub>	-5.407	24.7	70.7	95.4	18.3
145	b <sub>2g</sub>	-5.882	0.7	91.8	92.5	15.8
144	b <sub>2u</sub>	-6.078	0	64.2	64.2	73.5
143	e <sub>g</sub>	-6.09	2.1	63	65.1	66.9
142	e <sub>g</sub>	-6.09	2.1	63	65.1	66.9
141	a <sub>2u</sub>	-6.21	0.1	72.3	72.4	59.3
140	e <sub>g</sub>	-6.304	0	28.6	28.6	88.7
139	e <sub>g</sub>	-6.304	0	28.6	28.6	88.7
138	b <sub>1u</sub>	-6.325	0	20.7	20.7	94.1
137	e <sub>u</sub>	-6.359	0.2	93.8	94	18.4
136	e <sub>u</sub>	-6.359	0.2	93.8	94	18.4
135	a <sub>2u</sub>	-6.387	3.2	83.9	87.1	23
134	a <sub>1u</sub>	-6.821	0	44.6	44.6	79.6
133	a <sub>1g</sub>	-7.041	0.2	96.8	97	14.5
132	e <sub>g</sub>	-7.811	3.3	77.8	81.1	25.9
131	e <sub>g</sub>	-7.811	3.3	77.8	81.1	25.9
130	e <sub>u</sub>	-8.131	2.6	62.5	65.1	58.8

129	e <sub>u</sub>	-8.131	2.6	62.5	65.1	58.8
128	b <sub>1g</sub>	-8.131	1.6	43	44.6	87
127	b <sub>2u</sub>	-8.478	0	42.3	42.3	62.3
126	a <sub>1g</sub>	-8.483	0	30.8	30.8	89.2
125	e <sub>u</sub>	-8.498	4.7	58.8	63.4	52.6
124	e <sub>u</sub>	-8.498	4.7	58.8	63.4	52.6
123	a <sub>2g</sub>	-8.643	0	41.9	41.9	73.8
122	e <sub>u</sub>	-8.836	0	36.4	36.4	77.1
121	e <sub>u</sub>	-8.836	0	36.4	36.4	77.1
120	a <sub>2u</sub>	-8.861	0.3	35.9	36.3	85.3
119	e <sub>g</sub>	-8.882	2.4	48	50.4	68.4
118	e <sub>g</sub>	-8.882	2.4	48	50.4	68.4
117	a <sub>2g</sub>	-8.907	1.5	29.8	31.2	81.1
116	a <sub>1g</sub>	-9.4	63.9	28.6	92.5	13.5
115	b <sub>1u</sub>	-9.405	0	98.7	98.7	4.9
114	b <sub>1g</sub>	-9.916	17.6	39.6	57.1	65.7
113	b <sub>2g</sub>	-9.921	49.2	46	95.3	19.2

B3LYP

154	e <sub>g</sub>	-0.516	0	5.2	3.6	91.1
153	e <sub>g</sub>	-0.516	0	5.2	3.6	91.1
151	b <sub>2u</sub>	-0.823	0	19	0	81
150	b <sub>1u</sub>	-1.066	0	0	23.8	76.2
<b>149</b>	<b>e<sub>g</sub></b>	<b>-2.749</b>	<b>0</b>	<b>13.3</b>	<b>19</b>	<b>67.4</b>
<b>148</b>	<b>e<sub>g</sub></b>	<b>-2.749</b>	<b>0</b>	<b>13.3</b>	<b>19</b>	<b>67.4</b>
<b>147</b>	<b>a<sub>1u</sub></b>	<b>-4.936</b>	<b>0</b>	<b>0.1</b>	<b>0.1</b>	<b>99.8</b>
146	b <sub>1g</sub>	-6.652	0	53.8	0.9	25.1
145	b <sub>2u</sub>	-6.716	0	25.2	0	74.8
144	e <sub>g</sub>	-6.747	0	27.7	1.3	69.7
143	e <sub>g</sub>	-6.747	0	27.7	1.3	69.7
142	a <sub>2u</sub>	-6.772	0	6.2	39.7	53.9
141	e <sub>g</sub>	-6.942	0	0.7	10.1	89.2
140	e <sub>g</sub>	-6.942	0	0.7	10.1	89.2
139	b <sub>1u</sub>	-6.974	0	0	5.2	94.8
138	b <sub>2g</sub>	-7.028	0	12.3	61.6	25.6
137	a <sub>2u</sub>	-7.064	0	46.2	20.4	30.6
136	a <sub>1u</sub>	-7.501	0	0	0	100
135	e <sub>u</sub>	-7.512	0	18	50.2	31.6
134	e <sub>u</sub>	-7.512	0	18	50.2	31.6
133	a <sub>1g</sub>	-8.252	0	17.7	55.2	26.8
132	e <sub>g</sub>	-8.636	0	22.1	21.9	54.3
131	e <sub>g</sub>	-8.636	0	22.1	21.9	54.3
130	e <sub>u</sub>	-9.249	0.1	18.2	7.1	72.2
129	e <sub>u</sub>	-9.249	0.1	18.2	7.1	72.2
128	b <sub>1g</sub>	-9.284	0	1.1	2.9	94.5
127	b <sub>2u</sub>	-9.407	0	27.3	0	72.7
126	a <sub>1g</sub>	-9.639	0	1.7	3.2	95.2

125	e <sub>u</sub>	-9.659	0.1	32.5	2.8	60.8
124	e <sub>u</sub>	-9.659	0.1	32.5	2.8	60.8
123	a <sub>2g</sub>	-9.81	0	1.9	1.1	96.9
122	a <sub>2u</sub>	-9.829	0	7.5	3.7	88.4
121	e <sub>g</sub>	-9.85	0	2.7	13.7	82.7
120	e <sub>g</sub>	-9.85	0	2.7	13.7	82.7
PBE1PBE						
154	e <sub>g</sub>	-0.427	0.1	25.7	25.8	87.2
153	e <sub>g</sub>	-0.427	0.1	25.7	25.8	87.2
151	b <sub>2u</sub>	-0.739	0	37.4	37.4	65.6
150	b <sub>1u</sub>	-0.997	0	72.3	72.3	65.6
<b>149</b>	<b>e<sub>g</sub></b>	<b>-2.753</b>	<b>0.3</b>	<b>84.6</b>	<b>84.9</b>	<b>27.8</b>
<b>148</b>	<b>e<sub>g</sub></b>	<b>-2.753</b>	<b>0.3</b>	<b>84.6</b>	<b>84.9</b>	<b>27.8</b>
<b>147</b>	<b>a<sub>1u</sub></b>	<b>-5.133</b>	<b>0</b>	<b>71.2</b>	<b>71.2</b>	<b>32.9</b>
146	b <sub>1g</sub>	-7.026	19.9	75.7	95.6	16.9
145	b <sub>2u</sub>	-7.032	0	64.2	64.2	74.5
144	e <sub>g</sub>	-7.066	1.2	63.3	64.5	69.3
143	e <sub>g</sub>	-7.066	1.2	63.3	64.5	69.3
142	a <sub>2u</sub>	-7.079	0.2	77	77.2	50.6
141	e <sub>g</sub>	-7.26	0	28.5	28.5	88.4
140	e <sub>g</sub>	-7.26	0	28.5	28.5	88.4
139	b <sub>1u</sub>	-7.292	0	21	21	94.2
138	a <sub>2u</sub>	-7.377	2.4	80.5	82.9	31.5
137	b <sub>2g</sub>	-7.392	0.6	93.2	93.7	14
136	a <sub>1u</sub>	-7.831	0	40.9	40.9	82.9
135	e <sub>u</sub>	-7.898	0.2	94.5	94.8	17.4
134	e <sub>u</sub>	-7.898	0.2	94.5	94.8	17.4
133	a <sub>1g</sub>	-8.682	0.3	96.9	97.1	15.3
132	e <sub>g</sub>	-9.01	1.6	81.8	83.4	23.5
131	e <sub>g</sub>	-9.01	1.6	81.8	83.4	23.5
130	b <sub>1g</sub>	-9.583	1.4	42.8	44.2	87.4
129	e <sub>u</sub>	-9.586	1.6	60.1	61.7	63.1
128	e <sub>u</sub>	-9.586	1.6	60.1	61.7	63.1
127	b <sub>2u</sub>	-9.813	0	44.1	44.1	60.7
126	a <sub>1g</sub>	-9.947	0	30.2	30.2	89.7

a. HOMO is labeled in bold and LOMO are in bold italic.

**Supporting Information Table 4.** Gas-phase TDDFT predicted vertical excitation energies in PcZn using selected exchange-correlation functionals and molecular geometry optimized in gas-phase using B3LYP exchange-correlation functional.

transition	State Symm	E, eV	$f^a$	transitions and expansion coefficients <sup>b</sup>
------------	---------------	-------	-------	---

## BP86 exchange-correlation functional

1	E <sub>u</sub>	2.00	0.3202	135 → <b>148</b> , 0.10968; 141 → <b>148</b> , -0.20816; <b>147</b> → <b>149</b> , 0.57075
2	E <sub>u</sub>	2.00	0.3202	135 → <b>149</b> , 0.10968; 141 → <b>149</b> , -0.20816; <b>147</b> → <b>148</b> , -0.57075
3	E <sub>g</sub>	2.15	0	146 → <b>148</b> , 0.70154
4	E <sub>g</sub>	2.15	0	146 → <b>149</b> , 0.70154
5	E <sub>g</sub>	2.64	0	145 → <b>149</b> , 0.70043
6	E <sub>g</sub>	2.64	0	145 → <b>148</b> , 0.70043
7		2.88	0	142 → <b>149</b> , -0.48671; 143 → <b>148</b> , 0.48671
8	E <sub>u</sub>	2.88	0.0152	144 → <b>148</b> , 0.66675; 144 → <b>149</b> , 0.15928
9	E <sub>u</sub>	2.88	0.0152	144 → <b>148</b> , -0.15928; 144 → <b>149</b> , 0.66675
10		2.88	0	142 → <b>149</b> , 0.49036; 143 → <b>148</b> , 0.49036
11		2.90	0	142 → <b>148</b> , 0.48849; 143 → <b>149</b> , -0.48849
12		2.94	0	139 → <b>149</b> , -0.19850; 140 → <b>148</b> , -0.19850; 142 → <b>148</b> , 0.44456; 143 → <b>149</b> , 0.44456
13	B <sub>1g</sub>	3.00	0	139 → <b>149</b> , 0.32937; 140 → <b>148</b> , -0.32937; <b>147</b> → 150, 0.51595
14		3.03	0	139 → <b>148</b> , 0.49447; 140 → <b>149</b> , -0.49447
15		3.07	0	139 → <b>148</b> , 0.44891; 140 → <b>149</b> , 0.44891; <b>147</b> → 151, 0.29225
16		3.08	0	136 → <b>149</b> , -0.49926; 137 → <b>148</b> , 0.49926
17		3.09	0	136 → <b>148</b> , 0.49831; 137 → <b>149</b> , -0.49831
18	E <sub>u</sub>	3.09	0.0209	135 → <b>148</b> , 0.35302; 135 → <b>149</b> , 0.15221; 138 → <b>148</b> , -0.13862; 138 → <b>149</b> , -0.32150; 1 41 → <b>148</b> , 0.40998; 141 → <b>149</b> , 0.17677
19	E <sub>u</sub>	3.09	0.0209	135 → <b>148</b> , 0.15221; 135 → <b>149</b> , -0.35302; 138 → <b>148</b> , 0.32150; 138 → <b>149</b> , -0.13862; 141 → <b>148</b> , 0.17677; 141 → <b>149</b> , -0.40998
20	E <sub>u</sub>	3.15	0.1854	135 → <b>148</b> , -0.16099; 135 → <b>149</b> , 0.20686; 138 → <b>148</b> , 0.45151; 138 → <b>149</b> , -0.35138; 141 → <b>148</b> , -0.14475; 141 → <b>149</b> , 0.18600
21	E <sub>u</sub>	3.15	0.1854	135 → <b>148</b> , 0.20686; 135 → <b>149</b> , 0.16099; 138 → <b>148</b> , 0.35138; 138 → <b>149</b> , 0.45151; 141 → <b>148</b> , 0.18600; 141 → <b>149</b> , 0.14475
22		3.15	0	136 → <b>148</b> , 0.49278; 137 → <b>149</b> , 0.49278
23		3.16	0.0014	136 → <b>149</b> , 0.49094; 137 → <b>148</b> , 0.49094
24		3.21	0	139 → <b>149</b> , 0.43625; 140 → <b>148</b> , 0.43625; 142 → <b>148</b> , 0.17058; 143 → <b>149</b> , 0.17058
25	B <sub>2g</sub>	3.26	0	139 → <b>148</b> , -0.18747; 140 → <b>149</b> , -0.18747; <b>147</b> → 151, 0.61633
26	A <sub>2g</sub>	3.32	0	<b>147</b> → 152, 0.68725
27	B <sub>1g</sub>	3.40	0	139 → <b>149</b> , -0.34230; 140 → <b>148</b> , 0.34230; <b>147</b> → 150, 0.41018
28	E <sub>u</sub>	3.45	0.0857	134 → <b>148</b> , -0.25764; 134 → <b>149</b> , 0.13642; 135 → <b>148</b> , 0.14372; 135 → <b>149</b> , 0.27142;

29	E <sub>u</sub>	3.45	0.0857	141 → <b>148</b> , -0.11113; 141 → <b>149</b> , -0.20986; <b>147</b> → 154, 0.41327; <b>147</b> → 154, 0.21883 134 → <b>148</b> , -0.13642; 134 → <b>149</b> , -0.25764; 135 → <b>148</b> , -0.27142; 135 → <b>149</b> , 0.14372; 141 → <b>148</b> , 0.20986; 141 → <b>149</b> , -0.11113; <b>147</b> → 153, 0.41327; <b>147</b> → 154, 0.21883
30	E <sub>u</sub>	3.50	0.2654	134 → <b>148</b> , 0.11660; 134 → <b>149</b> , 0.32721; 135 → <b>148</b> , 0.22687; 138 → <b>149</b> , -0.11418; 141 → <b>148</b> , -0.17571; <b>147</b> → 153, 0.45217; <b>147</b> → 154, 0.16113
31	E <sub>u</sub>	3.50	0.2654	134 → <b>148</b> , 0.32721; 134 → <b>149</b> , -0.11660; 135 → <b>149</b> , -0.22687; 138 → <b>148</b> , 0.11418; 141 → <b>149</b> , 0.17571; <b>147</b> → 153, -0.16113; <b>147</b> → 154, 0.45217
32	A <sub>1u</sub>	3.54	0	146 → 150, 0.70629
33	A <sub>2u</sub>	3.80	0.0001	146 → 151, 0.70204
34	E <sub>g</sub>	3.81	0	133 → <b>148</b> , 0.69810
35	E <sub>g</sub>	3.81	0	133 → <b>149</b> , 0.69809
36	E <sub>u</sub>	3.82	0.481	134 → <b>148</b> , 0.49329; 135 → <b>149</b> , 0.26144; 140 → 150, 0.13316; 141 → <b>149</b> , -0.23438; <b>147</b> → 156; -0.12150
37	E <sub>u</sub>	3.82	0.481	134 → <b>149</b> , 0.49329; 135 → <b>148</b> , -0.26144; 139 → 150, -0.13316; 141 → <b>148</b> , 0.23438; <b>147</b> → 157, -0.12150
38	B <sub>2u</sub>	3.90	0	146 → 152, 0.70616
39	E <sub>g</sub>	4.04	0	146 → 154, 0.70540
40	E <sub>g</sub>	4.04	0	146 → 153, 0.70539
B3LYP exchange-correlation functional				
1	E <sub>u</sub>	2.09	0.4184	142 → <b>148</b> , -0.11660; 142 → <b>149</b> , -0.18316; <b>147</b> → <b>148</b> , -0.50749; <b>147</b> → <b>149</b> , 0.32307
2	E <sub>u</sub>	2.09	0.4184	142 → <b>148</b> , -0.18316; 142 → <b>149</b> , 0.11660; <b>147</b> → <b>148</b> , 0.32307; <b>147</b> → <b>149</b> , 0.50749
3	E <sub>g</sub>	3.04	0	146 → <b>148</b> , 0.70125
4	E <sub>g</sub>	3.04	0	146 → <b>149</b> , 0.70125
5		3.35	0	143 → <b>148</b> , 0.48514; 144 → <b>149</b> , -0.48514
6		3.35	0	143 → <b>148</b> , 0.49001; 144 → <b>149</b> , 0.49001
7	E <sub>u</sub>	3.39	0.0072	137 → <b>148</b> , 0.14890; 145 → <b>148</b> , 0.63504; 145 → <b>149</b> , -0.20700
8	E <sub>u</sub>	3.39	0.0072	137 → <b>149</b> , -0.14890; 145 → <b>148</b> , 0.20700; 145 → <b>149</b> , 0.63504
9	E <sub>g</sub>	3.45	0	138 → <b>148</b> , 0.69256
10	E <sub>g</sub>	3.45	0	138 → <b>149</b> , 0.69256
11	B <sub>lg</sub>	3.46	0	143 → <b>149</b> , -0.34904; 144 → <b>148</b> , 0.34904; <b>147</b> → 150, 0.47003
12	B <sub>lg</sub>	3.51	0	140 → <b>149</b> , 0.19272; 141 → <b>148</b> , -0.19272; 143 → <b>149</b> , 0.33865; 144 → <b>148</b> , -0.33865; <b>147</b> → 150, 0.42981

13		3.56	0	140 → <b>149</b> , -0.21810; 141 → <b>148</b> , -0.21810; 143 → <b>149</b> , 0.44048; 144 → <b>148</b> , 0.44048
14	B <sub>2g</sub>	3.62	0	140 → <b>148</b> , 0.19152; 141 → <b>149</b> , 0.19152; <b>147</b> → 151, 0.64122
15		3.65	0	140 → <b>148</b> , -0.49295; 141 → <b>149</b> , 0.49295; <b>147</b> → 152, 0.10692
16	E <sub>u</sub>	3.67	0.1971	137 → <b>148</b> , 0.39758; 137 → <b>149</b> , 0.12173; 139 → <b>149</b> , -0.17538; 142 → <b>148</b> , 0.47884; 142 → <b>149</b> , 0.14661; 145 → <b>148</b> , -0.12170
17	E <sub>u</sub>	3.67	0.1971	137 → <b>148</b> , -0.12173; 137 → <b>149</b> , 0.39758; 139 → <b>148</b> , -0.17538; 142 → <b>148</b> , -0.14661; 142 → <b>149</b> , 0.47884; 145 → <b>149</b> , 0.12170
18	A <sub>2g</sub>	3.74	0	<b>147</b> → 152, 0.68240
19	E <sub>u</sub>	3.75	0.3188	139 → <b>148</b> , 0.60270; 139 → <b>149</b> , -0.20779; 142 → <b>149</b> , 0.18457; <b>147</b> → 154, -0.15303
20	E <sub>u</sub>	3.75	0.3188	139 → <b>148</b> , 0.20779; 139 → <b>149</b> , 0.60270; 142 → <b>148</b> , 0.18457; <b>147</b> → 153, 0.15303
21		3.76	0	140 → <b>149</b> , 0.43074; 141 → <b>148</b> , 0.43074; 143 → <b>149</b> , 0.19821; 144 → <b>148</b> , 0.19821
22		3.78	0	140 → <b>148</b> , 0.45105; 141 → <b>149</b> , 0.45105; <b>147</b> → 151, -0.24575
23		3.82	0	140 → <b>149</b> , -0.43152; 141 → <b>148</b> , 0.43152; <b>147</b> → 150, 0.21804
24	E <sub>u</sub>	3.89	0.2959	<b>147</b> → 150, 0.21804; 136 → <b>149</b> , 0.24696; 137 → <b>148</b> , 0.43152; 137 → <b>149</b> , 0.19314; 139 → <b>149</b> , 0.13675; 142 → <b>148</b> , -0.28752; 142 → <b>149</b> , -0.12869; <b>147</b> → 153, -0.10238
25	E <sub>u</sub>	3.89	0.2959	136 → <b>148</b> , -0.24696; 136 → <b>149</b> , -0.11053; 137 → <b>148</b> , -0.19314; 137 → <b>149</b> , 0.43152; 139 → <b>148</b> , 0.13675; 142 → <b>148</b> , 0.12869; 142 → <b>149</b> , -0.28752; <b>147</b> → 154, 0.10238
26		3.92	0	134 → <b>149</b> , -0.49281; 135 → <b>148</b> , 0.49281
27		3.93	0	134 → <b>148</b> , -0.49710; 135 → <b>149</b> , 0.49710
28		3.94	0.0034	134 → <b>148</b> , 0.48181; 135 → <b>149</b> , 0.48181; 138 → 150, -0.12576
29		3.95	0	134 → <b>149</b> , 0.49017; 135 → <b>148</b> , 0.49017
30	E <sub>u</sub>	3.96	0.1468	<b>147</b> → 153, 0.38757; <b>147</b> → 154, 0.53449
31	E <sub>u</sub>	3.96	0.1468	<b>147</b> → 153, 0.53449; <b>147</b> → 154, -0.38757
32	E <sub>u</sub>	4.34	0.2024	136 → <b>148</b> , -0.16821; 136 → <b>149</b> , 0.59634; 137 → <b>148</b> , -0.15669; 142 → <b>148</b> , 0.13842
33	E <sub>u</sub>	4.34	0.2024	136 → <b>148</b> , 0.59634; 136 → <b>149</b> , 0.16821; 137 → <b>149</b> , 0.15669; 142 → <b>149</b> , -0.13842
34	E <sub>g</sub>	4.68	0	133 → <b>149</b> , 0.68383; 134 → 150, -0.10972
35	E <sub>g</sub>	4.68	0	133 → <b>148</b> , 0.68383; 135 → 150, -0.10972
36	A <sub>1u</sub>	4.84	0	146 → 150, 0.69022
37	A <sub>2g</sub>	5.02	0	<b>147</b> → 156, 0.69099

38	A <sub>2u</sub>	5.08	0.0001	146 → 151, 0.67989
39	A <sub>2g</sub>	5.13	0	131 → <b>149</b> , 0.32632; 132 → <b>148</b> , -0.32632; 145 → 150, 0.52317
40	E <sub>u</sub>	5.14	0.0227	140 → 150, 0.22877; 142 → 154, 0.12391; 143 → 150, 0.37668; 144 → 150, 0.11442; 144 → 151, -0.25087; 144 → 152, 0.16917; 145 → 154, -0.13786; <b>147</b> → 157, -0.10185; <b>147</b> → 158, 0.33529

PBE1PBE exchange-correlation functional

1	E <sub>u</sub>	2.12	0.4449	138 → <b>148</b> , -0.10359; 142 → <b>148</b> , 0.21451; <b>147</b> → <b>148</b> , 0.11239; <b>147</b> → <b>149</b> , 0.59785
2	E <sub>u</sub>	2.12	0.4449	138 → <b>149</b> , 0.10359; 142 → <b>149</b> , -0.21451; <b>147</b> → <b>148</b> , 0.59785; <b>147</b> → <b>149</b> , -0.11239
3	E <sub>g</sub>	3.18	0	146 → <b>148</b> , -0.31991; 146 → <b>149</b> , 0.62280
4	E <sub>g</sub>	3.18	0	146 → <b>148</b> , 0.62280; 146 → <b>149</b> , 0.31991
5		3.48	0	143 → <b>149</b> , -0.48320; 144 → <b>148</b> , 0.48320
6		3.48	0	143 → <b>149</b> , 0.48828; 144 → <b>148</b> , 0.48828
7	E <sub>u</sub>	3.52	0.0066	138 → <b>148</b> , -0.18608; 145 → <b>148</b> , 0.65071
8	E <sub>u</sub>	3.52	0.0066	138 → <b>149</b> , 0.18608; 145 → <b>149</b> , 0.65071
9	E <sub>g</sub>	3.58	0	137 → <b>148</b> , 0.61853; 137 → <b>149</b> , 0.31428
10	E <sub>g</sub>	3.58	0	137 → <b>148</b> , -0.31428; 137 → <b>149</b> , 0.61853
11	B <sub>1g</sub>	3.59	0	143 → <b>148</b> , -0.24453; 144 → <b>149</b> , 0.24453; <b>147</b> → 150, 0.58269
12		3.66	0	140 → <b>149</b> , 0.16373; 141 → <b>148</b> , -0.16373; 143 → <b>148</b> , -0.41566; 144 → <b>149</b> , 0.41566; <b>147</b> → 150, -0.30015
13		3.73	0	140 → <b>149</b> , -0.22881; 141 → <b>148</b> , -0.22881; 143 → <b>148</b> , 0.43526; 144 → <b>149</b> , 0.43526
14	B <sub>2g</sub>	3.75	0	140 → <b>148</b> , 0.13900; 141 → <b>149</b> , 0.13900; <b>147</b> → 151, 0.66432
15		3.81	0	140 → <b>148</b> , 0.49220; 141 → <b>149</b> , -0.49220; <b>147</b> → 152, 0.10870
16	E <sub>u</sub>	3.83	0.2598	138 → <b>148</b> , 0.38072; 138 → <b>149</b> , 0.14531; 139 → <b>149</b> , -0.14666; 142 → <b>148</b> , 0.47317; 142 → <b>149</b> , 0.18060; 145 → <b>148</b> , 0.14710
17	E <sub>u</sub>	3.83	0.2598	138 → <b>148</b> , -0.14531; 138 → <b>149</b> , 0.38072; 139 → <b>148</b> , -0.14666; 142 → <b>148</b> , -0.18060; 142 → <b>149</b> , 0.47317; 145 → <b>149</b> , -0.14710
18	A <sub>2g</sub>	3.89	0	<b>147</b> → 152, 0.68257
19	E <sub>u</sub>	3.90	0.4561	138 → <b>149</b> , -0.11759; 139 → <b>148</b> , 0.60203; 142 → <b>149</b> , 0.24239; <b>147</b> → 154, 0.15253
20	E <sub>u</sub>	3.90	0.4561	138 → <b>148</b> , -0.11759; 139 → <b>149</b> , 0.60203; 142 → <b>148</b> , 0.24239; <b>147</b> → 153, -0.15253
21		3.91	0	140 → <b>149</b> , 0.42429; 141 → <b>148</b> , 0.42429; 143 → <b>148</b> , 0.21101; 144 → <b>149</b> , 0.21101
22		3.96	0	140 → <b>148</b> , 0.47026; 141 → <b>149</b> , 0.47026;

23		3.96	0	<b>147</b> → 151, -0.17381 140 → <b>149</b> , -0.44287; 141 → <b>148</b> , 0.44287; 143 → <b>148</b> , -0.10364; 144 → <b>149</b> , 0.10364; <b>147</b> → 150, -0.16333
24	E <sub>u</sub>	4.01	0.2129	136 → <b>149</b> , -0.20802; 138 → <b>148</b> , 0.42443; 138 → <b>149</b> , -0.19891; 139 → <b>148</b> , -0.11633; 139 → <b>149</b> , 0.24823; 142 → <b>148</b> , -0.25935; 142 → <b>149</b> , 0.12154; 145 → <b>148</b> , 0.11963
25	E <sub>u</sub>	4.01	0.2129	136 → <b>148</b> , 0.20802; 138 → <b>148</b> , 0.19891; 138 → <b>149</b> , 0.42443; 139 → <b>148</b> , 0.24823; 139 → <b>149</b> , 0.11633; 142 → <b>148</b> , -0.12154; 145 → <b>149</b> , -0.11963
26		4.08	0.0039	134 → <b>149</b> , 0.47605; 135 → <b>148</b> , 0.47605; 137 → 150, -0.15178
27		4.08	0	134 → <b>148</b> , -0.49016; 135 → <b>149</b> , 0.49016
28	E <sub>u</sub>	4.09	0.106	139 → <b>148</b> , -0.10902; <b>147</b> → 154, 0.67049
29	E <sub>u</sub>	4.09	0.106	139 → <b>149</b> , 0.10902; <b>147</b> → 153, 0.67049
30		4.09	0	134 → <b>149</b> , -0.49575; 135 → <b>148</b> , 0.49575
31		4.10	0	134 → <b>148</b> , 0.48759; 135 → <b>149</b> , 0.48759
32	E <sub>u</sub>	4.50	0.1637	136 → <b>148</b> , 0.54505; 136 → <b>149</b> , 0.32232; 138 → <b>149</b> , -0.12179; 142 → <b>149</b> , 0.10748
33	E <sub>u</sub>	4.50	0.1637	136 → <b>148</b> , -0.32232; 136 → <b>149</b> , 0.54505; 138 → <b>148</b> , 0.12179; 142 → <b>148</b> , -0.10748
34	E <sub>g</sub>	4.87	0	133 → <b>148</b> , 0.66286; 133 → <b>149</b> , 0.12311; 134 → 150, -0.13228
35	E <sub>g</sub>	4.87	0	133 → <b>148</b> , 0.12311; 133 → <b>149</b> , -0.66286; 135 → 150, 0.13228
36	A <sub>1u</sub>	5.08	0	128 → <b>149</b> , -0.10018; 129 → <b>148</b> , 0.10018; 146 → 150, 0.67686
37	A <sub>1g</sub>	5.25	0	139 → 150, -0.20153; 142 → 152, -0.17095; 143 → 154, -0.17527; 144 → 153, -0.17527; 145 → 151, -0.27755; <b>147</b> → 155, 0.52336
38	A <sub>2g</sub>	5.27	0	131 → <b>149</b> , -0.19028; 132 → <b>148</b> , 0.19028; <b>147</b> → 158, 0.65019
39	E <sub>u</sub>	5.30	0.0635	141 → 150, 0.23488; 142 → 153, 0.14917; 143 → 150, 0.15827; 144 → 151, -0.27855; 144 → 152, 0.21103; 145 → 153, -0.18953; <b>147</b> → 156, 0.44676
40	E <sub>u</sub>	5.30	0.0634	140 → 150, -0.23487; 142 → 154, -0.14925; 143 → 151, -0.27856; 143 → 152, -0.21095; 144 → 150, -0.15871; 145 → 154, -0.18943; <b>147</b> → 157, 0.44665

---

a. Oscillator strength; b. HOMO and LUMO are labeled in bold.



**Supporting Information Table 5.** Calculated vertical excitation energies and oscillator strengths of PcZn using 14 exchange-correlation functionals and gas-phase molecular geometry optimized using B3LYP exchange-correlation functional.

X $\alpha$			LSDA			BP86		
state symm	E, eV	<i>f</i>	state symm	E, eV	<i>f</i>	state symm	E, eV	<i>f</i>
E <sub>u</sub>	2.01	0.3155	E <sub>u</sub>	2.01	0.3164	E <sub>u</sub>	2	0.3202
E <sub>u</sub>	2.01	0.3154	E <sub>u</sub>	2.01	0.3164	E <sub>u</sub>	2	0.3202
E <sub>g</sub>	2.1	0	E <sub>g</sub>	2.07	0	E <sub>g</sub>	2.15	0
E <sub>g</sub>	2.1	0	E <sub>g</sub>	2.07	0	E <sub>g</sub>	2.15	0
E <sub>g</sub>	2.56	0	E <sub>g</sub>	2.55	0	E <sub>g</sub>	2.64	0
E <sub>g</sub>	2.56	0	E <sub>g</sub>	2.55	0	E <sub>g</sub>	2.64	0
E <sub>u</sub>	2.86	0.0154		2.85	0		2.88	0
E <sub>u</sub>	2.86	0.0154	E <sub>u</sub>	2.85	0.0152	E <sub>u</sub>	2.88	0.0152
	2.86	0	E <sub>u</sub>	2.85	0.0152	E <sub>u</sub>	2.88	0.0152
	2.86	0		2.86	0		2.88	0
	2.87	0		2.87	0		2.9	0
	2.92	0		2.92	0		2.94	0
	2.98	0		2.98	0	B <sub>1g</sub>	3	0
B <sub>1g</sub>	2.99	0		2.99	0		3.03	0
	3	0	B <sub>1g</sub>	3	0		3.07	0
	3.01	0		3	0		3.08	0
	3.05	0		3.04	0		3.09	0
	3.06	0		3.06	0	E <sub>u</sub>	3.09	0.0209
	3.07	0.0015	E <sub>u</sub>	3.07	0.0139	E <sub>u</sub>	3.09	0.0209
E <sub>u</sub>	3.07	0.0133	E <sub>u</sub>	3.07	0.0139	E <sub>u</sub>	3.15	0.1854
E <sub>u</sub>	3.07	0.0133		3.07	0.0015	E <sub>u</sub>	3.15	0.1854
E <sub>u</sub>	3.13	0.2029	E <sub>u</sub>	3.12	0.1987		3.15	0
E <sub>u</sub>	3.13	0.2029	E <sub>u</sub>	3.12	0.1987		3.16	0.0014
	3.19	0		3.19	0		3.21	0
B <sub>2g</sub>	3.27	0	B <sub>2g</sub>	3.27	0	B <sub>2g</sub>	3.26	0
A <sub>2g</sub>	3.29	0	A <sub>2g</sub>	3.33	0	A <sub>2g</sub>	3.32	0
B <sub>1g</sub>	3.39	0	B <sub>1g</sub>	3.39	0	B <sub>1g</sub>	3.4	0
E <sub>u</sub>	3.46	0.1006	E <sub>u</sub>	3.46	0.142	E <sub>u</sub>	3.45	0.0857
E <sub>u</sub>	3.46	0.1006	E <sub>u</sub>	3.46	0.142	E <sub>u</sub>	3.45	0.0857
A <sub>1u</sub>	3.49	0	A <sub>1u</sub>	3.47	0	E <sub>u</sub>	3.5	0.2654
E <sub>u</sub>	3.5	0.2151	E <sub>u</sub>	3.51	0.1715	E <sub>u</sub>	3.5	0.2654
E <sub>u</sub>	3.5	0.2151	E <sub>u</sub>	3.51	0.1715	A <sub>1u</sub>	3.54	0
E <sub>g</sub>	3.69	0	E <sub>g</sub>	3.68	0	A <sub>2u</sub>	3.8	0.0001
E <sub>g</sub>	3.69	0	E <sub>g</sub>	3.68	0	E <sub>g</sub>	3.81	0
A <sub>2u</sub>	3.75	0.0001	A <sub>2u</sub>	3.73	0.0001	E <sub>g</sub>	3.81	0
B <sub>2u</sub>	3.81	0	B <sub>2u</sub>	3.82	0	E <sub>u</sub>	3.82	0.481
E <sub>u</sub>	3.82	0.491	E <sub>u</sub>	3.82	0.5103	E <sub>u</sub>	3.82	0.481
E <sub>u</sub>	3.82	0.491	E <sub>u</sub>	3.82	0.5103	B <sub>2u</sub>	3.9	0

E <sub>g</sub>	3.99	0	E <sub>g</sub>	3.97	0	E <sub>g</sub>	4.04	0
E <sub>g</sub>	3.99	0	E <sub>g</sub>	3.97	0	E <sub>g</sub>	4.04	0
BPW91			BLYP			VSXC		
state symm	E, eV	<i>f</i>	state symm	E, eV	<i>f</i>	state symm	E, eV	<i>f</i>
E <sub>u</sub>	2	0.3207	E <sub>u</sub>	1.99	0.3151	E <sub>u</sub>	2.04	0.3529
E <sub>u</sub>	2	0.3207	E <sub>u</sub>	1.99	0.3151	E <sub>u</sub>	2.04	0.3529
E <sub>g</sub>	2.15	0	E <sub>g</sub>	2.18	0	E <sub>g</sub>	2.57	0
E <sub>g</sub>	2.15	0	E <sub>g</sub>	2.18	0	E <sub>g</sub>	2.57	0
E <sub>g</sub>	2.62	0	E <sub>g</sub>	2.66	0	E <sub>g</sub>	2.93	0
E <sub>g</sub>	2.62	0	E <sub>g</sub>	2.66	0	E <sub>g</sub>	2.93	0
	2.88	0		2.87	0	E <sub>u</sub>	3.01	0.0147
E <sub>u</sub>	2.88	0.0151	E <sub>u</sub>	2.87	0.0152	E <sub>u</sub>	3.01	0.0147
E <sub>u</sub>	2.88	0.0151	E <sub>u</sub>	2.87	0.0152		3.02	0
	2.88	0		2.87	0		3.02	0
	2.9	0		2.88	0		3.04	0
	2.94	0		2.93	0		3.09	0
B <sub>1g</sub>	3	0	B <sub>1g</sub>	2.99	0	B <sub>1g</sub>	3.11	0
	3.03	0		3.02	0		3.16	0
	3.07	0		3.05	0		3.19	0
	3.07	0	E <sub>u</sub>	3.08	0.0247	E <sub>u</sub>	3.23	0.0137
	3.08	0	E <sub>u</sub>	3.08	0.0247	E <sub>u</sub>	3.23	0.0137
E <sub>u</sub>	3.09	0.0225		3.08	0	E <sub>u</sub>	3.29	0.2434
E <sub>u</sub>	3.09	0.0225		3.1	0	E <sub>u</sub>	3.29	0.2434
	3.14	0	E <sub>u</sub>	3.13	0.1862		3.35	0
E <sub>u</sub>	3.15	0.1779	E <sub>u</sub>	3.13	0.1862	B <sub>2g</sub>	3.36	0
E <sub>u</sub>	3.15	0.1779		3.15	0	A <sub>2g</sub>	3.37	0
	3.15	0.0014		3.16	0.0015		3.37	0
	3.21	0		3.2	0		3.39	0
B <sub>2g</sub>	3.26	0	B <sub>2g</sub>	3.24	0		3.44	0
A <sub>2g</sub>	3.34	0	A <sub>2g</sub>	3.28	0		3.45	0.0017
B <sub>1g</sub>	3.4	0	B <sub>1g</sub>	3.39	0	B <sub>1g</sub>	3.52	0
E <sub>u</sub>	3.45	0.1177	E <sub>u</sub>	3.44	0.0708	E <sub>u</sub>	3.57	0.0004
E <sub>u</sub>	3.45	0.1177	E <sub>u</sub>	3.44	0.0708	E <sub>u</sub>	3.57	0.0004
E <sub>u</sub>	3.5	0.2437	E <sub>u</sub>	3.48	0.2736	E <sub>u</sub>	3.64	0.3394
E <sub>u</sub>	3.5	0.2437	E <sub>u</sub>	3.48	0.2736	E <sub>u</sub>	3.64	0.3394
A <sub>1u</sub>	3.54	0	A <sub>1u</sub>	3.57	0	E <sub>u</sub>	3.97	0.4883
E <sub>g</sub>	3.8	0	E <sub>g</sub>	3.8	0	E <sub>u</sub>	3.97	0.4883
E <sub>g</sub>	3.8	0	E <sub>g</sub>	3.8	0	A <sub>1u</sub>	4.03	0
A <sub>2u</sub>	3.8	0.0001	E <sub>u</sub>	3.8	0.4699	E <sub>g</sub>	4.13	0
E <sub>u</sub>	3.82	0.4842	E <sub>u</sub>	3.8	0.4699	E <sub>g</sub>	4.13	0
E <sub>u</sub>	3.82	0.4842	A <sub>2u</sub>	3.82	0.0001	A <sub>2u</sub>	4.28	0.0002
B <sub>2u</sub>	3.91	0	B <sub>2u</sub>	3.9	0	B <sub>2u</sub>	4.35	0
E <sub>g</sub>	4.04	0	E <sub>g</sub>	4.07	0	A <sub>2u</sub>	4.42	0.0021
E <sub>g</sub>	4.04	0	E <sub>g</sub>	4.07	0	A <sub>2g</sub>	4.5	0

B3LYP			B3P86			B3PW91		
state symm	E, eV	<i>f</i>	state symm	E, eV	<i>f</i>	state symm	E, eV	<i>f</i>
E <sub>u</sub>	2.09	0.4184	E <sub>u</sub>	2.1	0.4236	E <sub>u</sub>	2.1	0.4229
E <sub>u</sub>	2.09	0.4184	E <sub>u</sub>	2.1	0.4236	E <sub>u</sub>	2.1	0.4229
E <sub>g</sub>	3.04	0	E <sub>g</sub>	3.02	0	E <sub>g</sub>	3	0
E <sub>g</sub>	3.04	0	E <sub>g</sub>	3.02	0	E <sub>g</sub>	3	0
	3.35	0		3.36	0		3.36	0
	3.35	0		3.36	0		3.36	0
E <sub>u</sub>	3.39	0.0072	E <sub>u</sub>	3.39	0.0074	E <sub>u</sub>	3.4	0.0078
E <sub>u</sub>	3.39	0.0072	E <sub>u</sub>	3.39	0.0074	E <sub>u</sub>	3.4	0.0078
E <sub>g</sub>	3.45	0	E <sub>g</sub>	3.43	0	E <sub>g</sub>	3.41	0
E <sub>g</sub>	3.45	0	E <sub>g</sub>	3.43	0	E <sub>g</sub>	3.41	0
B <sub>1g</sub>	3.46	0	B <sub>1g</sub>	3.47	0	B <sub>1g</sub>	3.47	0
B <sub>1g</sub>	3.51	0	B <sub>1g</sub>	3.52	0	B <sub>1g</sub>	3.52	0
	3.56	0		3.57	0		3.57	0
B <sub>2g</sub>	3.62	0	B <sub>2g</sub>	3.64	0	B <sub>2g</sub>	3.64	0
	3.65	0		3.65	0		3.66	0
E <sub>u</sub>	3.67	0.1971	E <sub>u</sub>	3.68	0.1701	E <sub>u</sub>	3.68	0.1671
E <sub>u</sub>	3.67	0.1971	E <sub>u</sub>	3.68	0.1701	E <sub>u</sub>	3.68	0.1671
A <sub>2g</sub>	3.74	0	E <sub>u</sub>	3.75	0.3241	E <sub>u</sub>	3.76	0.3295
E <sub>u</sub>	3.75	0.3188	E <sub>u</sub>	3.75	0.3241	E <sub>u</sub>	3.76	0.3294
E <sub>u</sub>	3.75	0.3188		3.77	0		3.77	0
	3.76	0	A <sub>2g</sub>	3.79	0		3.79	0
	3.78	0		3.79	0	A <sub>2g</sub>	3.8	0
	3.82	0		3.83	0		3.83	0
E <sub>u</sub>	3.89	0.2959	E <sub>u</sub>	3.9	0.3291	E <sub>u</sub>	3.89	0.3351
E <sub>u</sub>	3.89	0.2959	E <sub>u</sub>	3.9	0.3291	E <sub>u</sub>	3.89	0.3351
	3.92	0		3.91	0		3.9	0
	3.93	0		3.92	0		3.91	0
	3.94	0.0034		3.93	0.0033		3.92	0.0033
	3.95	0		3.94	0		3.93	0
E <sub>u</sub>	3.96	0.1468	E <sub>u</sub>	3.97	0.1375	E <sub>u</sub>	3.98	0.1333
E <sub>u</sub>	3.96	0.1468	E <sub>u</sub>	3.97	0.1375	E <sub>u</sub>	3.98	0.1333
E <sub>u</sub>	4.34	0.2024	E <sub>u</sub>	4.35	0.21	E <sub>u</sub>	4.35	0.2069
E <sub>u</sub>	4.34	0.2024	E <sub>u</sub>	4.35	0.21	E <sub>u</sub>	4.35	0.2069
E <sub>g</sub>	4.68	0	E <sub>g</sub>	4.69	0	E <sub>g</sub>	4.68	0
E <sub>g</sub>	4.68	0	E <sub>g</sub>	4.69	0	E <sub>g</sub>	4.68	0
A <sub>1u</sub>	4.84	0	A <sub>1u</sub>	4.83	0	A <sub>1u</sub>	4.81	0
A <sub>2g</sub>	5.02	0	A <sub>2u</sub>	5.08	0.0001	A <sub>2u</sub>	5.06	0.0001
A <sub>2u</sub>	5.08	0.0001	A <sub>1g</sub>	5.13	0	A <sub>1g</sub>	5.13	0
A <sub>2g</sub>	5.13	0	A <sub>2g</sub>	5.15	0	A <sub>2g</sub>	5.15	0
E <sub>u</sub>	5.14	0.0227	E <sub>u</sub>	5.16	0.013	E <sub>u</sub>	5.16	0.0131
PBE1PBE			B98			BHandH		

state symm	E, eV	<i>f</i>	state symm	E, eV	<i>f</i>	state symm	E, eV	<i>f</i>
E <sub>u</sub>	2.12	0.4449	E <sub>u</sub>	2.1	0.4301	E <sub>u</sub>	2.1	0.526
E <sub>u</sub>	2.12	0.4449	E <sub>u</sub>	2.1	0.4301	E <sub>u</sub>	2.1	0.526
E <sub>g</sub>	3.18	0	E <sub>g</sub>	3.13	0		3.95	0
E <sub>g</sub>	3.18	0	E <sub>g</sub>	3.13	0		3.96	0
	3.48	0		3.41	0	B <sub>1g</sub>	3.96	0
	3.48	0		3.41	0	E <sub>u</sub>	4.02	0.0003
E <sub>u</sub>	3.52	0.0066	E <sub>u</sub>	3.44	0.0068	E <sub>u</sub>	4.02	0.0003
E <sub>u</sub>	3.52	0.0066	E <sub>u</sub>	3.44	0.0068	E <sub>g</sub>	4.11	0
E <sub>g</sub>	3.58	0	B <sub>1g</sub>	3.52	0	E <sub>g</sub>	4.11	0
E <sub>g</sub>	3.58	0	E <sub>g</sub>	3.52	0	B <sub>2g</sub>	4.2	0
B <sub>1g</sub>	3.59	0	E <sub>g</sub>	3.52	0	A <sub>2g</sub>	4.24	0
	3.66	0		3.57	0		4.31	0
	3.73	0		3.63	0	E <sub>u</sub>	4.33	1.1984
B <sub>2g</sub>	3.75	0	B <sub>2g</sub>	3.67	0	E <sub>u</sub>	4.33	1.1984
	3.81	0		3.71	0		4.4	0
E <sub>u</sub>	3.83	0.2598	E <sub>u</sub>	3.74	0.2147	E <sub>g</sub>	4.41	0
E <sub>u</sub>	3.83	0.2598	E <sub>u</sub>	3.74	0.2147	E <sub>g</sub>	4.41	0
A <sub>2g</sub>	3.89	0		3.81	0	E <sub>u</sub>	4.5	0.016
E <sub>u</sub>	3.9	0.4561	A <sub>2g</sub>	3.81	0.3717	E <sub>u</sub>	4.5	0.016
E <sub>u</sub>	3.9	0.4561	E <sub>u</sub>	3.81	0.3717		4.51	0
	3.91	0	E <sub>u</sub>	3.82	0		4.52	0
	3.96	0		3.85	0		4.57	0
	3.96	0		3.88	0	E <sub>u</sub>	4.59	0.0583
E <sub>u</sub>	4.01	0.2129	E <sub>u</sub>	3.93	0.281	E <sub>u</sub>	4.59	0.0583
E <sub>u</sub>	4.01	0.2129	E <sub>u</sub>	3.93	0.281	E <sub>u</sub>	4.66	0.0258
	4.08	0.0039		4.01	0	E <sub>u</sub>	4.66	0.0258
	4.08	0	E <sub>u</sub>	4.01	0.1286		4.73	0
E <sub>u</sub>	4.09	0.106	E <sub>u</sub>	4.01	0.1286		4.79	0.007
E <sub>u</sub>	4.09	0.106		4.02	0.0036		4.88	0
	4.09	0		4.02	0		4.96	0
	4.1	0		4.03	0		5.03	0
E <sub>u</sub>	4.5	0.1637	E <sub>u</sub>	4.41	0.1849	E <sub>u</sub>	5.16	0.0567
E <sub>u</sub>	4.5	0.1637	E <sub>u</sub>	4.41	0.1849	E <sub>u</sub>	5.16	0.0567
E <sub>g</sub>	4.87	0	E <sub>g</sub>	4.79	0	A <sub>1u</sub>	5.32	0
E <sub>g</sub>	4.87	0	E <sub>g</sub>	4.79	0	A <sub>2g</sub>	5.33	0
A <sub>1u</sub>	5.08	0	A <sub>1u</sub>	4.97	0	E <sub>g</sub>	5.7	0
A <sub>1g</sub>	5.25	0	A <sub>2g</sub>	5.16	0	E <sub>g</sub>	5.7	0
A <sub>2g</sub>	5.27	0	A <sub>1g</sub>	5.17	0	A <sub>1g</sub>	5.76	0
E <sub>u</sub>	5.3	0.0635	A <sub>2u</sub>	5.2	0	E <sub>u</sub>	5.83	0.1103
E <sub>u</sub>	5.3	0.0634	A <sub>2g</sub>	5.22	0	E <sub>u</sub>	5.83	0.1103
BHandHLYP			HF					
state symm	E, eV	<i>f</i>	state symm	E, eV	<i>f</i>			
E <sub>u</sub>	2.06	0.523	E <sub>u</sub>	1.58	0.598			

E <sub>u</sub>	2.06	0.523	E <sub>u</sub>	1.58	0.598			
B <sub>1g</sub>	3.92	0	B <sub>1g</sub>	4.3	0			
	3.95	0	A <sub>2g</sub>	4.42	0			
	3.96	0	B <sub>2g</sub>	4.49	0			
E <sub>u</sub>	4.02	0	E <sub>u</sub>	4.7	0.1314			
E <sub>u</sub>	4.02	0	E <sub>u</sub>	4.7	0.1314			
B <sub>2g</sub>	4.16	0		4.74	0			
A <sub>2g</sub>	4.23	0	B <sub>2g</sub>	4.9	0			
E <sub>g</sub>	4.24	0	E <sub>u</sub>	5.04	1.1825			
E <sub>g</sub>	4.24	0	E <sub>u</sub>	5.04	1.1825			
	4.31	0	A <sub>1u</sub>	5.17	0			
E <sub>u</sub>	4.33	1.1952		5.22	0			
E <sub>u</sub>	4.33	1.1952	E <sub>u</sub>	5.26	0.0339			
	4.4	0	E <sub>u</sub>	5.26	0.0339			
E <sub>u</sub>	4.5	0.0119		5.3	0			
E <sub>u</sub>	4.5	0.0119	E <sub>u</sub>	5.42	0.0751			
E <sub>g</sub>	4.5	0	E <sub>u</sub>	5.42	0.0751			
E <sub>g</sub>	4.5	0	A <sub>2g</sub>	5.48	0			
	4.52	0		5.78	0			
	4.53	0		5.85	0			
E <sub>u</sub>	4.56	0.0679		5.85	0			
E <sub>u</sub>	4.56	0.0679	E <sub>g</sub>	5.86	0			
	4.58	0	E <sub>g</sub>	5.86	0			
E <sub>u</sub>	4.67	0.035	E <sub>u</sub>	5.93	0.3861			
E <sub>u</sub>	4.67	0.035	E <sub>u</sub>	5.93	0.3861			
	4.74	0		6.03	0.0124			
	4.86	0.0072	E <sub>g</sub>	6.06	0			
	4.96	0	E <sub>g</sub>	6.06	0			
	5.04	0		6.23	0			
	5.11	0		6.29	0			
E <sub>u</sub>	5.16	0.0513	E <sub>u</sub>	6.46	0.1146			
E <sub>u</sub>	5.16	0.0513	E <sub>u</sub>	6.46	0.1146			
A <sub>2g</sub>	5.3	0	B <sub>1g</sub>	6.47	0			
A <sub>1u</sub>	5.31	0		6.62	0			
A <sub>1g</sub>	5.72	0	A <sub>1g</sub>	6.69	0			
E <sub>g</sub>	5.78	0	E <sub>g</sub>	6.74	0			
E <sub>g</sub>	5.78	0	E <sub>g</sub>	6.74	0			
E <sub>u</sub>	5.8	0.0955	E <sub>u</sub>	6.88	0.4889			
E <sub>u</sub>	5.8	0.0955	E <sub>u</sub>	6.88	0.4887			

**Supporting Information Table 6.** Gas-phase predicted vertical excitation energies of PcZn using semi-empirical methods and molecular geometry optimized in gas-phase using B3LYP exchange-correlation functional.

Transition	State Symmetry	E, cm <sup>-1</sup>	<i>f</i> <sup>a</sup>	Transitions and expansion coefficients <sup>b</sup>	
PM3					
1	1 <sup>1</sup> E <sub>u</sub>	15.26	0.3771	<b>93</b> → <b>94</b>	0.611395
2	2 <sup>1</sup> E <sub>u</sub>	36.65	0.3129	<b>93</b> → 98	-0.590780
3	3 <sup>1</sup> E <sub>u</sub>	30.30	0.2562	89 → <b>95</b>	0.531525
4	5 <sup>1</sup> E <sub>u</sub>	32.29	2.5335	92 → <b>95</b>	0.464926
5	6 <sup>1</sup> E <sub>u</sub>	38.40	0.0280	86 → <b>94</b>	-0.587522
6	1 <sup>1</sup> A <sub>2u</sub>	34.08	0.0129	82 → <b>94</b>	-0.337521
				81 → <b>95</b>	-0.337521
7	7 <sup>1</sup> E <sub>u</sub>	35.00	0.6876	85 → <b>94</b>	0.402211
8	8 <sup>1</sup> E <sub>u</sub>	36.65	0.3129	<b>93</b> → 98	-0.590780
9		39.71	0.0012	92 → 101	0.707093
ZINDO/S 0.585					
1	1 <sup>1</sup> E <sub>u</sub>	14.18	1.0926	<b>93</b> → <b>94</b>	0.602406
2	2 <sup>1</sup> E <sub>u</sub>	27.51	0.0214	<b>93</b> → 98	0.697548
3	3 <sup>1</sup> E <sub>u</sub>	33.28	0.1307	91 → <b>94</b>	-0.469716
4	4 <sup>1</sup> E <sub>u</sub>	34.19	0.0405	<b>93</b> → 102	-0.553328
5	5 <sup>1</sup> E <sub>u</sub>	35.14	2.5545	92 → <b>94</b>	-0.546581
6	6 <sup>1</sup> E <sub>u</sub>	36.90	0.1544	86 → <b>94</b>	0.454317
7	1 <sup>1</sup> A <sub>2u</sub>	38.83	0.0126	81 → <b>94</b>	0.447782
				80 → <b>95</b>	-0.447782
ZINDO/S 0.640					
1	1 <sup>1</sup> E <sub>u</sub>	15.21	1.1695	<b>93</b> → <b>94</b>	-0.665390
2	2 <sup>1</sup> E <sub>u</sub>	29.59	0.0227	<b>93</b> → 98	0.699389
3	3 <sup>1</sup> E <sub>u</sub>	35.58	0.1073	91 → <b>94</b>	-0.580758
4	4 <sup>1</sup> E <sub>u</sub>	36.58	0.5603	<b>93</b> → 102	0.564939
5	5 <sup>1</sup> E <sub>u</sub>	37.37	2.3371	92 → <b>94</b>	-0.603996
6	1 <sup>1</sup> A <sub>2u</sub>	39.53	0.0127	81 → <b>95</b>	-0.343024
				80 → <b>94</b>	0.343024
7	6 <sup>1</sup> E <sub>u</sub>	39.68	0.1171	86 → <b>94</b>	-0.514792
ZINDO/S 0.649					
1	1 <sup>1</sup> E <sub>u</sub>	15.37	1.1813	<b>93</b> → <b>94</b>	0.575521
				<b>93</b> → <b>95</b>	0.369870
2	2 <sup>1</sup> E <sub>u</sub>	29.92	0.0229	<b>93</b> → 98	0.691856
3	3 <sup>1</sup> E <sub>u</sub>	35.92	0.0990	91 → <b>94</b>	-0.543088
4	4 <sup>1</sup> E <sub>u</sub>	36.96	0.7131	<b>93</b> → 102	-0.571428
5	5 <sup>1</sup> E <sub>u</sub>	37.73	2.2257	92 → <b>94</b>	-0.596692
6	1 <sup>1</sup> A <sub>2u</sub>	39.64	0.0128	81 → <b>95</b>	-0.393674
				80 → <b>94</b>	-0.393674

a. Oscillator strength; b. HOMO and LUMO are labeled in bold.